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The development and application of a novel hazard scoring tool for assessing impacts of cosmetic ingredients on aquatic ecosystems: A case study of rinse-off cosmetics

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Abstract

The cosmetic industry has been committed to promoting less hazardous products to reduce the environmental impacts of cosmetic ingredients. This requires identifying safer cosmetic ingredients for developing cosmetic formulations that are less harmful to the environment. However, one of the challenges in developing eco-friendly cosmetics relies on integrating all environmental hazard (EH) information of cosmetic ingredients to select the most eco-friendly ones (i.e., ingredients least harmful to the aquatic environment). Thus, we developed a hazard scoring tool (IARA matrix), which integrates data on biodegradation, bioaccumulation, and acute aquatic toxicity, providing a hazard index to classify cosmetic ingredients (raw materials) into categories of EH (low, moderate, high, or very high). The classification of the IARA was based on parameters established by Cradle to Cradle (C2C), the US Environmental Protection Agency (USEPA), and European Regulation 1272/2008, considering the most conservative values of each source. The Leopold matrix was employed as a model for the tool, using a numerical scale from 0 to 6 (lowest to highest EH). According to the IARA, we have successfully demonstrated that ultraviolet (UV) filter ingredients have the highest EH out of 41 cosmetic ingredients commonly used for rinse-off products. In addition to UV filters, triclosan (bactericide) and dimethicone (emollient) presented the second-highest EH for aquatic ecosystems, and humectants presented the lowest hazard index. By applying the IARA in the case study of rinse-off products, we have estimated that the aquatic hazard of cosmetic products can be reduced 46% by identifying less hazardous ingredients and combining them into a cosmetic formulation. In summary, the IARA tool allows the estimation of the EH of cosmetic ingredients, provides safer products, and helps achieve sustainability for cosmetic products. *Integr Environ Assess Manag* 2023;00:1–17. © 2023 SETAC

KEYWORDS: Aquatic toxicology; Cosmetics; Eco-friendly products; Environmental toxicology; Scoring rank tool

INTRODUCTION

Personal care products (PCPs) are products intended for external use on the human body (Brausch & Rand, 2011). The production and consumption of PCPs in large quantities and inefficient sewage and/or water treatment result in frequent detection of PCP ingredients in aquatic environments (Balakrishna et al., 2017; Brausch & Rand, 2011; Cuderman & Heath, 2007; Ebele et al., 2017; Fu et al., 2019). The removal efficiency of PCP ingredients by conventional sewage and/or water treatment is affected by several factors related to a chemical, such as the chemical nature (W. Li et al., 2015), physicochemical properties (Evgenidou et al., 2015; W. Li et al., 2015; Luo et al., 2014), biodegradability (Jones et al., 2005), and antimicrobial properties that may cause toxicity to activated sludge bacteria or alter microbial community (Dann & Hontela, 2011; Drury et al., 2013). Thus, several cosmetic ingredients from PCPs are poorly eliminated by conventional treatment, such as the activated sludge process (Y. Yang et al., 2017). Additionally, the ineffective policy during the product life cycle and poor consumer habits also contribute to the entrance of PCP ingredients into aquatic environments (Dreher et al., 2022).

Some ingredients of PCPs can harm aquatic life, resulting in negative consequences for aquatic ecosystems (Dreher et al., 2022). Preservatives (e.g., antimicrobial agents), humectants (e.g., moisturizing agents), surfactants (e.g., cleaning agents), and ultraviolet (UV) filters have caused toxicity to aquatic organisms, such as invertebrates (*Daphnia magna*, *Ceriodaphnia dubia*; Bazin et al., 2010; Brausch et al., 2007;

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Orvos et al., 2002; Terasaki et al., 2009), fish (*Pimephales promelas, Orizias latipis, Oncorhynchus mykiss, Danio rerio, Lepomis macrochirus*; Dobbins et al., 2009; Horie et al., 2018; Kim et al., 2009; Orvos et al., 2002), and algae (*Pseudokirchneriella subcapitata, Scenedesmus subspicatus*; L. H. Yang et al., 2008). The type of toxic effect varies depending on the cosmetic ingredient present in the PCPs. For instance, endocrine disruption (Chavoshani et al., 2020; Kwon & Choi, 2021), teratogenic effects, reproductive toxicity (Baran et al., 2021; Horie et al., 2018; Sarmah et al., 2020), genotoxicity (Binelli et al., 2009; Capkin et al., 2017), and neurotoxicity (Closset et al., 2021; M. Li et al., 2018) have been reported on aquatic organisms as a result of exposure to cosmetic ingredients present in PCPs. These cosmetic ingredients can also bioaccumulate in aquatic organisms (Y. Yang et al., 2017); consequently, they may cause biomagnification within aquatic food webs (Bhattacharya, 2016; Peng et al., 2017).

Based on the evidence of hazards caused by PCP ingredients, authorities and the cosmetic industry are increasingly expressing concern about the environmental safety of PCP ingredients, particularly those applied on rinse-off cosmetic products and products used in recreational waters (e.g., sunscreens). In addition, society has increased concern about environmental pollution, demanding environmental protection from toxic substances (Amberg & Fogarassy, 2019). Therefore, the cosmetic industry must find ways to achieve and develop eco-friendly cosmetics (in this study, "eco-friendly" refers to chemicals less hazardous to the aquatic environment).

The protection of the aquatic environment requires environmental hazard (EH) and risk assessments. Thus, aquatic toxicity data of chemicals is often required by European Union (EU) REACH Regulation (Registration, Evaluation, Authorisation and Restriction of Chemicals). The aquatic toxicity of chemicals is determined by organisms representing the three trophic levels: algae or plants (primary producers), invertebrates (e.g., crustaceans such as *Daphnia* spp.; primary consumers and/or secondary producers), and vertebrates (usually fish; then on a secondary level, consumers). The REACH also requires biodegradation and bioaccumulation data of chemicals.

For cosmetics, legal requirements regarding EH assessment vary depending on the country. In Brazil and the United States (US), assessing the EH of cosmetics is not required in product registration (Ferreira et al., 2022), whereas in the EU, under REACH, a persistent, bioaccumulative and toxic (PBT)/very persistent and very bioaccumulative (vPvB) assessment is required for those substances manufactured or imported in amounts equal to or greater than 10 tonnes/year (European Chemicals Agency, n.d.). However, sunscreens pose a unique challenge in international harmonization because they are considered cosmetics according to China, Japan, Brazil, and the EU, whereas under US law, they are considered over-the-counter drugs; in this case, UV filters are strictly regulated by the Food and Drug Administration according to pharma requirements (Ferreira et al., 2022). Furthermore, the cosmetic industry represents one of the most challenging industrial sectors to apply new protective actions to environmental policies because it must be aligned with the current legislation banning animal testing in cosmetics (EU Regulation 1223/2009; Rio de Janeiro regulation 7814/17). Several animal-free alternatives have been proposed to predict the EH of cosmetic ingredients and products. Thus, besides in vitro and in silico methods, an integrated data analysis strategy in weight of evidence approaches is currently under discussion (Lillicrap et al., 2020; Moe et al., 2020), and integrated approaches that gather information from different endpoints and test methods to assess EH have been recommended (Paparella et al., 2021).

This study developed a hazard scoring tool, known as the IARA matrix (*Índice de Avaliação de Risco Ambiental*), based on the Leopold matrix (Leopold, 1971). The IARA integrates data on biodegradation, bioaccumulation, and aquatic toxicity from databases or nonanimal tests to classify cosmetic ingredients into four categories of aquatic hazard: low, moderate, high, and very high. The IARA matrix attributes scores to each cosmetic ingredient. By using the ingredient scores, it is possible to calculate the formulation index (FI), compare different cosmetic formulations, and choose the lowest hazard option for the environment (eco-friendly product). The applicability of the IARA to identifying safer cosmetic ingredients and developing cosmetic products with reduced aquatic hazard was evaluated here by a case study of rinse-off cosmetics. By developing this tool, we aimed to contribute to the sustainability of cosmetics and promote nonanimal testing approaches to aquatic hazard assessment.

MATERIALS AND METHODS

An integrated data analysis strategy to assess the EH of cosmetics to aquatic ecosystems: the IARA matrix

The IARA matrix (*Índice de Avaliação de Risco Ambiental*, Grupo Boticário, São José dos Pinhais-PR/Brazil) was a tool developed to predict the environmental hazard of cosmetics to aquatic ecosystems. The matrix integrates data on biodegradation, bioaccumulation, and acute aquatic toxicity, and a quantitative classification with a numerical scale (score) from 0 (lowest aquatic hazard) to 6 (highest aquatic hazard), based on the Leopold matrix (Leopold, 1971), is applied to each of these parameters, classifying them according to their aquatic hazard. Then, for each cosmetic ingredient, an environmental hazard index is determined by the sum of the parameters' score. Finally, the EH index of ingredients can be used to evaluate cosmetic formulations regarding the EH of the product by calculating the FI. The FI is the total aquatic hazard attributed to a cosmetic formulation and is obtained by considering the concentration of the ingredient in the formula, the active ingredient percentage, and the EH index of each ingredient contained in the cosmetic formulation. The detailed process of developing the IARA matrix is described in the following subsections.

Defining hazard categorization of biodegradation, bioaccumulation, and acute aquatic toxicity parameters

Parameters of biodegradation, bioaccumulation, and aquatic toxicity are important to assess the EH and risk of chemicals according to international regulations; however, hazard classification varies among authorities. Thus, the hazard classifications were defined from a literature search, in which we reviewed documents from the most recognized databases and governmental and accreditation bodies (EU: CosIng—Cosmetic Ingredients and Substances; ECHA—European Chemicals Agency; REACH—Registration, Evaluation, Authorisation and Restriction of Chemicals; European Regulation 1272/2008 (Regulation (EC), 2008); OECD—Organisation for Economic Co-operation and Development; IUCLID International Uniform Chemical Information Database. UK: EA—Environment Agency. Australia: AICIS—Australian Industrial Chemicals Introduction Scheme. USA: PubChem; NIOSH—National Institute for Occupational Safety and Health; C2C—Cradle to Cradle; EPA—Environmental Protection Agency. The chosen sources for the IARA matrix were EPA, C2C, and European Regulation 1272/2008), which are well-known hazard classifications adopted by many countries from the EU, North America, and Latin America, including Brazil.

After that, we compared the classification values established for biodegradation, bioaccumulation, and acute aquatic toxicity of EPA (Office of Pollution Prevention and Toxics & US Environmental Protection Agency [USEPA], 2011), C2C (Cradle to Cradle, 2012), and European Regulation 1272/2008 (Regulation [EC] No. 1272/2008 of the European Parliament and of the Council on classification, 2008; Supporting Information: Table S1) and selected the most conservative value of each parameter described in these guidelines (i.e., the classification that represented the most protective values for the environment) to be applied in the IARA matrix.

Based on the most conservative classification values (Supporting Information: Table S1), the EPA values were selected for the biodegradation parameter; the C2C values were adopted for the bioaccumulation parameter; EPA and C2C values were used for acute aquatic toxicity because they are equivalent (Table 1). Additionally, the "very high" hazard classification selected from EPA was adopted (Table 1).

Attributing scores to parameters of biodegradation, bioaccumulation, and aquatic toxicity to calculate the EH index of cosmetic ingredients

The IARA matrix was developed based on an adaptation of the Leopold matrix. The Leopold matrix is a valuable method for assessing environmental impacts in civil engineering works (e.g., roads, airports, railways). The rows of this matrix represent environmental issues, and columns stand for the activities identified as causing an environmental impact. A ranking value (magnitude and/or importance) is determined for each interaction (Leopold, 1971). For the IARA, a ranking value was applied to each hazard classification (biodegradation, bioaccumulation, and aquatic toxicity; Table 1). Then, a numerical scale from 0 to 6 was determined by dividing by two the hazard classification values and attributing scores to each range of the classification values: low (0–1); moderate (2–3); high (4–5); very high (6; Table 2).

In the stage of creating a cosmetic formula, the cosmetic ingredients can be assessed by the IARA matrix, and for that, the environmental data (biodegradation, bioaccumulation, and acute aquatic toxicity) of the substances under evaluation are added to the matrix, and a score is attributed to each parameter. The sum of the scores results in a final score for the substance: the EH index, an index that integrates the data on biodegradation, bioaccumulation, and aquatic toxicity. The EH index ranges from 0 to 18. For instance, if the cosmetic ingredient yields 6 (highest score) for each parameter, the EH index will be 18. The EH index can be used to classify cosmetic ingredients regarding their aquatic hazard, identifying the safer ingredients for a cosmetic formulation.

Determining the FI by the IARA matrix to develop eco-friendly cosmetic products

The EH index values can be used to develop cosmetic formulations with lower EH by determining ingredient indexes (II) and comparing FI. The EH index is the aquatic hazard index for each raw material obtained by integrating data on

TABLE 1 Ranking adaptation used in the IARA matrix based on classification criteria of EPA, C2C, and European Regulation 1272/2008

Hazard	Biodegradation	Bioaccumulation	Acute aquatic toxicity[a] (LC50/EC50)
Low	T1/2 > 16 days > 70%	BCF < 100 or	>100 mg/L
		Log K_{ow} < 2	
Moderate	T1/2 16–60 days	BCF 100–500 or	10–100 mg/L
		Log K_{ow} < 3–2	
High	T1/2 > 60 days	BCF > 500 or	<10 mg/L
		Log K_{ow} > 3	
Very high	T1/2 > 180 days	BCF > 5000,1	<1 mg/L

Abbreviations: BCF, bioconcentration factor; EC50, half maximal effect concentration; LC50, half maximal lethal concentration; Log K_{ow}, octanol–water partition coefficient; T1/2, half-life of substances.
[a]Valid for fish (96 h), *Daphnia* (46 h) or algae (72 h).

TABLE 2 Aquatic hazard assessment by the IARA matrix

Hazard	Boundaries	Biodegradation T1/2 (days)	Bioaccumulation BCF	Bioaccumulation Log K_{ow}	Acute aquatic toxicity LC50/EC50 (mg/L)	Score
Low	0–1	0–8	<10	<1.0	>500.1	0
		8.1–16	10.1–100	1.1–2	100.1–500	1
Moderate	2–3	16.1–30	100.1–250	2.1–2.5	50.1–100	2
		30.1–60	250.1–500	2.6–3.0	10.1–50	3
High	4–5	60.1–120	500.1–2000	3.1–3.7	5.1–10	4
		120.1–180	2000.1–5000	3.8–6.0	1.1–5	5
Very high	6	>180.1	>5000.1	-	<1	6

Abbreviations: BCF, bioconcentration factor; EC50, half maximal effect concentration; LC50, half maximal lethal concentration; Log K_{ow}, octanol–water partition coefficient; T1/2, half-life of substances.

biodegradation, bioaccumulation, and aquatic toxicity of an ingredient (raw material) in the IARA matrix, as explained above. The II is the index attributed to each ingredient, now, however, considering its use in developing a cosmetic formulation. Thus, the II is calculated considering the EH index, the concentration used in the formulation (percentage), and the active ingredient percentage. For that, the EH index of each cosmetic ingredient is multiplied by their respective concentration (percentage) in the product formulation (i.e., the ingredient amount in the formulation, which is set at 100%), and by the active ingredient concentration (percentage; i.e., the percentage of a chemical substance in a solution). The value obtained is converted to a decimal and divided by 100. The final result is the ingredient index (II) of the cosmetic ingredient. The FI is the final aquatic hazard attributed to a cosmetic formulation, and the sum of the II indexes of all ingredients present in the formulation calculates it. The mathematical formulas to calculate II and FI are:

$$\textit{Ingredient index } (II) = \left(\frac{a \times b \times c}{100}\right) \div 100,$$

where *a* is the EH index, *b* the concentration of the cosmetic ingredient in the formula (%), and *c* the active ingredient of the cosmetic ingredient (%).

$$\textit{Formula index } (FI) = \sum_{i=1}^{n} II_i = II_1 + II_2 + II_3 + \cdots + II_n.$$

When comparing formulations, the lowest FI indicates the cosmetic formulation with the lowest aquatic hazard. Thus, the FI integrates the EH index of cosmetic ingredients allowing the selection of the cosmetic formulation with the lowest aquatic EH among several product candidates during stages of product development.

Evaluating the applicability of the IARA matrix to predict the EH of cosmetic ingredients and to help develop eco-friendly cosmetic products

To verify the applicability of the IARA matrix in classifying cosmetic ingredients by their EH, 41 cosmetic ingredients used in rinse-off products were selected and evaluated by this method. After that, some of the cosmetic ingredients studied were selected to compose formulations, and by the calculation of the FI, the applicability of the IARA matrix in developing eco-friendly cosmetic products was demonstrated. These evaluations of cosmetic ingredients and cosmetic formulations are described in the following subsections.

Hazard classification of cosmetic ingredients by the IARA matrix

First, a list of cosmetic ingredients commonly used in rinse-off cosmetic products was selected to be evaluated by the matrix (Table 3). Then, the required environmental data for the evaluation were obtained from scientific studies and databases (AICIS, ECHA, IUCLID, Pubchem, and CONCAWE). The criteria for considering data from scientific studies were to use the data from OECD methods recognized by accreditation and/or regulatory bodies. When the data were not available in literature or databases, in silico analysis (EPI Suite-Estimation Program Interface and ALTOX) or the OECD test methods 301B/1992 (biodegradation test) (OECD, 1992), 107/1995 (partition coefficient—bioaccumulation test) (OECD, 1995), and 201/2011 (growth inhibition test in algae) (OECD, 2011) were performed. Therefore, no new animal testing was performed due to cosmetic company policies and in accordance with the increasing efforts to ban animal testing in the cosmetic industry since the EU Regulation No. 1223/2009.

Developing eco-friendly cosmetic products using the IARA matrix

To demonstrate the applicability of the IARA matrix in developing eco-friendly cosmetic products, we selected some of the evaluated ingredients to develop shampoo formulations (Supporting Information: Table S4). Using the EH index obtained by the IARA matrix of the selected ingredients for the shampoo formulation, the ingredient indexes (II) and FI were determined. The percentage difference in aquatic EH between the shampoo formulations could be verified by comparing the FI, which drives the decision of the most eco-friendly formulation.

TABLE 3 Selected cosmetic ingredients from rinse-off products

Cosmetic ingredient (INCI name)	CAS number	Function
Acrylates copolymer	25133-97-5	Antistatic/film former
Polyquaternium-7	25590-05-6	Antistatic/film former
Cetyl palmitate	540-10-3	Emollient
Dibutyl adipate	105-99-7	Emollient/film former
Glycol distearate	627-83-8	Emollient/emulsifier/viscosity controller
Isododecane	31807-55-3	Emollient/solvent
Dimethicone	63148-62-9	Emollient
Octyldodecanol	5333-42-6	Emollient
Paraffinum liquidum (mineral oil)	8012-95-1	Emollient/solvent
Sodium astrocaryum murumuruate	-	Emollient/surfactant
Vitis vinifera grape seed oil	85594-37-2	Emollient/skin conditioner
Acrylates/C10-30 alkyl acrylate cross-polymer	-	Emulsion stabilizer/film former/ viscosity controller
Triethanolamine	102-71-6	pH regulator
Benzyl alcohol	100-51-6	Preservative
Cetrimonium chloride	112-02-7	Preservative/surfactant/antistatic
Phenoxyethanol	122-99-6	Preservative
Triclosan	3380-34-5	Preservative/bactericide
Butyrospermum parkii (shea butter)	194043-92-0	Skin conditioner/viscosity controller
Glycerin	56-81-5	Skin protector/humectant
Hexylene glycol	107-41-5	Skin conditioner/solvent
Panthenol	81-13-0	Skin conditioner
Persea gratissima oil	8024-32-6	Skin conditioner
Propylene glycol	57-55-6	Skin conditioner/humectant
Ricinus communis seed oil	8001-79-4	Skin conditioner
Sorbitol	50-70-4	Skin conditioner/humectant
C13-C15 alkane	64742-46-7	Solvent
Benzophenone-3	131-57-7	UV filter
Butyl methoxydibenzoylmethane	70356-09-1	UV filter
Ethylhexyl methoxycinnamate	5466-77-3	UV filter
Ethylhexyl salicylate	118-60-5	UV filter
Homosalate	118-56-9	UV filter
Octocrylene	6197-30-4	UV filter
Titanium dioxide (CI 77891)	13463-67-7	UV filter/dye/opacifier
Cocamidopropyl betaine	61789-40-0	Surfactant/antistatic
Sodium cocoamphoacetate	90387-76-1	Surfactant
Cocamide DIPA	68855-69-6	Surfactant

(*Continued*)

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TABLE 3 (*Continued*)

Cosmetic ingredient (INCI name)	CAS number	Function
Disodium laureth sulfosuccinate	68815-56-5	Surfactant
Sodium laureth sulfate	3088-31-1	Surfactant
Sodium laureth sulfate/disodium laureth sulfosuccinate	3088-31-1/39354-45-5	Surfactant
Sodium lauryl sulfate	151-21-3	Surfactant
Stearyl alcohol	112-92-5	Surfactant/emulsifier/viscosity controller

Abbreviations: CAS number, Chemical Abstracts Service number; INCI, International Nomenclature Cosmetic Ingredient.

RESULTS

The environmental data (bioaccumulation, biodegradation, and acute aquatic toxicity) of the cosmetic ingredients evaluated in this study are presented in Supporting Information: Table S2. Table 4 shows their EH assessed by the IARA matrix clustered according to their function in cosmetic products. In Table 5, the overall rank of the EH of these cosmetic ingredients can be verified.

The results from the IARA revealed that UV filters presented the highest EH index out of 41 cosmetic ingredients evaluated (Table 5). Among the UV filters evaluated, butyl methoxydibenzoylmethane and octocrylene were the ingredients of greatest concern, exhibiting the highest EH index (16), whereas titanium dioxide presented the lowest EH index (1) of this group of cosmetic ingredients. Conditioners/humectants had the lowest EH indexes among the cosmetic ingredients, representing the ingredient group least hazardous to aquatic environments. Four out of eight ingredients from this group displayed scores of 0, and *Butyrospermum parkii* (shea butter) presented the highest EH index (5) due to its higher bioaccumulation capacity (3—moderate). For preservatives and antimicrobial agents, triclosan presented the highest EH index (14), whereas phenoxyethanol was of least concern to aquatic ecosystems (EH index of 1). Dimethicone and paraffinum liquidum were the most hazardous ingredients of the emollients group (EH index of 13 and 11, respectively) due to their high bioaccumulation potential (6 and 5—very high and high) and low biodegradability (6—very high). *Vitis vinifera* grape seed oil and cetyl palmitate represent the least concerning emollient ingredients, with an EH index of 4. For the surfactants group, Cocamide DIPA was the most hazardous surfactant (EH index of 9), classified in the high category of aquatic toxicity (5) and only moderate biodegradability (4—moderate). The surfactants sodium cocoamphoacetate, sodium laureth sulfate, and sodium lauryl sulfate surfactants were of the least concern of EH, with an EH index of 4.

An overall ranking of EH for all the evaluated cosmetic ingredients is elaborated and described in Table 5. The cosmetic ingredients are organized in descending order of EH, and some cosmetic ingredients share the same rank because of equal EH index values. The overall rank demonstrated that octocrylene (UV filter), butyl methoxydibenzoylmethane (UV filter), and triclosan (antimicrobial agent) are in the three first positions on the list with the highest EH index values.

Two shampoo formulations were developed using the IARA data to demonstrate the applicability of this hazard classification tool in developing eco-friendly cosmetic products. Using the IARA data in product development achieved a reduction in the EH of cosmetic products on aquatic ecosystems. The shampoo formulations A and B presented FIs of 1.26 and 2.36, respectively, and the comparison of these FIs indicates that the shampoo formulation A is 46% more eco-friendly than formulation B because it presents reduced aquatic hazard according to the IARA matrix (Table 6).

DISCUSSION

Development of the environmental impact assessment and scoring system: the IARA matrix

The cosmetic industry has been committed to taking to heart the principles of sustainable development. For that, this industry sector has taken several actions to integrate the principles of sustainable development into all stages of the product life cycle, that is, from conception and product development to consumer use (Hitce et al., 2018). With respect to their commitment to improving environmental protection, many in the cosmetic industry have moved toward more eco-friendly product formulations by integrating Green Chemistry principles, such as principle 4, which addresses safer chemicals (Hitce et al., 2018; Lackmann et al., 2021). However, identifying safer and greener ingredients to develop eco-friendly cosmetic products has been a challenge for the cosmetic industry for several reasons: lack of environmental data for cosmetics, exclusive adoption of animal-free testing, and the lack of a quantitative scientific methodology to integrate environmental data for scoring cosmetic ingredients regarding their hazard. Growing efforts to develop industry-wide environmental impact assessment and scoring systems have been recently verified (Hitce et al., 2018), and until today, there is no system dedicated to this purpose published or freely available for use. Thus, in this study, we present the IARA matrix—an EH assessment and scoring system—that integrates the main criteria for aquatic impacts determined by international agencies (EPA, European Regulation 1272/

TABLE 4 The aquatic hazard of cosmetic ingredients used in rinse-off products and assessed by the IARA matrix

Cosmetic ingredient	Biodegradation	Bioaccumulation	Acute aquatic toxicity	EH index
Antistatics/film formers				
Acrylates copolymer	6	0	1	7
Polyquaternium-7	6	0	6	12
Emollients				
Cetyl palmitate	1	0	3	4
Dimethicone	6	6	1	13
Dibutyl adipate	0	5	3	8
Glycol distearate	1	5	0	6
Isododecane	1	4	1	6
Octyldodecanol	2	4	1	7
Paraffinum liquidum (mineral oil)	6	4	1	11
Sodium astrocaryum murumuruate	0	5	3	8
Vitis vinifera grape seed oil	0	3	1	4
Emulsion stabilizer				
Acrylates/C10-30 alkyl acrylate cross-polymer	6	1	1	8
pH regulator				
Triethanolamine	0	0	3	3
Preservatives/antimicrobial agents				
Benzyl alcohol	1	1	1	3
Phenoxyethanol	1	0	0	1
Triclosan	3	5	6	14
Conditioners/humectants				
Butyrospermum parkii (shea butter)	1	3	1	5
Glycerin	0	0	0	0
Hexylene glycol	1	0	0	1
Panthenol	0	0	0	0
Persea gratissima oil	0	0	2	2
Propylene glycol	0	0	0	0
Ricinus communis seed oil	2	0	1	3
Sorbitol	0	0	0	0
Solvent				
C13-C15 alkane	3	2	3	8
UV filters				
Benzophenone-3	2	2	5	9
Butyl methoxydibenzoylmethane	6	4	6	16
Ethylhexyl methoxycinnamate	1	3	6	10
Ethylhexyl salicylate	1	2	0	3
Homosalate	2	2	6	10

(*Continued*)

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TABLE 4 (*Continued*)

Cosmetic ingredient	Biodegradation	Bioaccumulation	Acute aquatic toxicity	EH index
Octocrylene	6	4	6	16
Titanium dioxide (CI 77891)	0	0	1	1
Surfactants				
Cetrimonium chloride	6	1	6	13
Cocamidopropyl betaine	0	0	4	4
Sodium cocoamphoacetate	1	0	3	4
Sodium laureth sulfate	1	0	3	4
Sodium laureth sulfate/disodium laureth sulfosuccinate	0	1	3	4
Cocamide DIPA	4	0	5	9
Sodium lauryl sulfate	1	0	3	4
Disodium laureth sulfosuccinate	2	0	5	7
Stearyl alcohol	0	2	1	3

Note: The scores of biodegradability, bioaccumulation, and acute aquatic toxicity represent the following hazard boundaries: low (0–1); moderate (2–3), high (4–5), and very high (6).
Abbreviation: EH, environmental hazard.

2008, and C2C), aiming to design finished products with favorable green scores (i.e., reduced EH).

Other tools and computer software applications that evaluate the hazards of cosmetic ingredients are currently available (e.g., Think Dirty, INCI Beauty, Yuka, Skin Deep scoring systems). However, unlike the IARA, they generally assess and score the hazards of cosmetic ingredients based on human health data, such as endpoints of carcinogenicity, skin irritation, skin sensitization, and reproductive and developmental toxicity. Moreover, in general, the purposes of these tools or apps differ from those of the IARA, such as informing and educating consumers about safer choices related to potential harm to human health. Particular consideration should be given to the Sustainable Product Optimization Tool (SPOT) developed by L'Oréal; different from the others mentioned above, this tool considers environmental data. However, this encompasses other aspects of product development and production (e.g., renewable material, packaging, social impacts) to perform life cycle assessment and reduce the environmental footprint of their products (L'Oréal, n.d.), thus, also differing from the IARA matrix. The GAIA (Global Aquatic Ingredient Assessment) by Johnson & Johnson and EcoSun Pass by BASF are tools closer to the idea of the IARA matrix; they address the EH, including aquatic hazard; however, they are also not identical to the IARA. EcoSun Pass by BASF is a methodology specially developed to assess the environmental impact of sunscreen formulations by an integrated approach considering information on aquatic toxicity, biodegradation, LogPow, bioaccumulation, sediment toxicity, terrestrial toxicity, and endocrine disruption (*EcoSun Pass—BASF*, n.d.). This tool is not freely available, and customers can test their products by hiring a service. Global Aquatic Ingredient Assessment, like the IARA matrix, has a developmental concept integrating data on biodegradation, bioaccumulation, and toxicity of algae and fish. The GAIA scores raw materials from 0 to 100 using data from a multitude of internal and external sources, including peer-reviewed scientific studies and government databases, and, unlike the IARA matrix, persistence is weighted higher because rapid degradation limits the effects of bioaccumulation and ecotoxicity (Global Aquatic Ingredient Assessment [GAIA]—J&J Consumer Health, 2021). However, because GAIA is not freely available and concepts of development are not fully disclosed, a detailed comparison with the IARA cannot be made.

Here, it is important to address a limitation of obtaining aquatic toxicity data from public databases because the available acute toxicity data do not always have a concordance with test species, and it is known that algae, invertebrates, and fish may have different sensitivity depending on the type of test substance (Barron et al., 2021; Kienzler et al., 2019; Tebby et al., 2011; Teixidó et al., 2020; Wei et al., 2006). In a study comparing the acute toxicity data of *Daphnia*, fish and algae using more than 600 substances, the potential classification derived from the three tests was identical in 45.2% of the substances (Weyers et al., 2000). Fish and *Daphnia* were reported to have the highest correlation (Tebby et al., 2011; Weyers et al., 2000), and either fish or *Daphnia* tests would lead to a similar classification (Weyers et al., 2000). In this study, we collected aquatic toxicity data from databases, which vary in species, and when data were not available for a cosmetic ingredient, the algal growth inhibition test (OECD TG 201) was performed. The algal toxicity test was chosen to be applied in

TABLE 5 Overall rank of aquatic hazard of cosmetic ingredients from rinse-off products classified by the IARA matrix

Ranking	Cosmetic ingredient	Biodegradation	Bioaccumulation	Acute aquatic toxicity	EH index
1°	Octocrylene	6	4	6	16
-	Butyl methoxydibenzoylmethane	6	4	6	16
2°	Triclosan	3	5	6	14
3°	Dimethicone	6	6	1	13
-	Cetrimonium chloride	6	1	6	13
4°	Polyquaternium-7	6	0	6	12
5°	Paraffinum liquidum (mineral oil)	6	4	1	11
6°	Ethylhexyl methoxycinnamate	1	3	6	10
-	Homosalate	2	2	6	10
7°	Cocamide DIPA	4	0	5	9
-	Benzophenone-3	2	2	5	9
8°	Acrylates/C10-30 alkyl acrylate cross-polymer	6	1	1	8
-	C13–C15 alkane	3	2	3	8
-	Dibutyl adipate	0	5	3	8
-	Sodium astrocaryum murumuruate	0	5	3	8
9°	Acrylates copolymer	6	0	1	7
-	Disodium laureth sulfosuccinate	2	0	5	7
-	Octyldodecanol	2	4	1	7
10°	Isododecane	1	4	1	6
-	Glycol distearate	1	5	0	6
11°	*Butyrospermum parkii* (shea butter)	1	3	1	5
12°	Cetyl palmitate	1	0	3	4
-	*Vitis vinifera* grape seed oil	0	3	1	4
-	Cocamidopropyl betaine	0	0	4	4
-	Sodium laureth sulfate/disodium laureth sulfosuccinate	0	1	3	4
-	Sodium laureth sulfate	1	0	3	4
-	Sodium lauryl sulfate	1	0	3	4
-	Sodium cocoamphoacetate	1	0	3	4
13°	Stearyl alcohol	0	2	1	3
-	Benzyl alcohol	1	1	1	3
-	*Ricinus communis* seed oil	2	0	1	3
-	Ethylhexyl salicylate	1	2	0	3
-	Triethanolamine	0	0	3	3
14°	*Persea gratissima* Oil	0	0	2	2
15°	Titanium dioxide (CI 77891)	0	0	1	1
-	Hexylene glycol	1	0	0	1
-	Phenoxyethanol	1	0	0	1

(*Continued*)

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TABLE 5 (*Continued*)

Ranking	Cosmetic ingredient	Biodegradation	Bioaccumulation	Acute aquatic toxicity	EH index
16°	Glycerin	0	0	0	0
-	Sorbitol	0	0	0	0
-	Propylene glycol	0	0	0	0
-	Panthenol	0	0	0	0

Abbreviations: EH, environmental hazard; -, ingredients that have the same rank position.

the IARA matrix because of our company policy of not using any type of animal test to assess our products.

Another important limitation related to the data gap for aquatic toxicity is that the IARA matrix does not consider long-term effects, such as chronic toxicity. Although chronic toxicity provides more restrictive values of effects on aquatic organisms, the data gap for chronic toxicity is greater than for acute aquatic toxicity of cosmetic ingredients. Additionally, there is a greater limit of available nonanimal test methods for chronic toxicity than for acute toxicity, making it challenging to fill data gaps for the use of chronic toxicity in the IARA matrix. This has limited the consideration of chronic data in the IARA matrix so far because it could increase uncertainties in classifying cosmetic ingredients by this tool and in developing eco-friendly cosmetic products that require the comparison of cosmetic formulations.

The three parameters integrated into the IARA matrix (biodegradation, bioaccumulation, acute aquatic toxicity) were considered equally important to predicting aquatic hazard, and thus equal scores were given to these parameters. This decision was based on environmental premises that led to assigning equal importance to the three parameters. These environmental premises refer to previous studies demonstrating the interconnection of the three parameters, which can be mutually dependent and important in an EH decision. Leonards et al. (2011) studied the impact of biodegradation on toxicity and bioaccumulation of refinery effluents and concluded that the three criteria are related. A biodegradation step reduced the number of bioaccumulative substances and toxicity to levels comparable with the control samples. This example demonstrates the importance of combining persistence, bioaccumulation, and toxicity tests in assessing the hazard of substances in effluents. For instance, if an ingredient with low biodegradability (0), high potential for bioaccumulation (5), and very high acute toxicity (6) is compared with a second ingredient that has a very high biodegradability (6), high potential for bioaccumulation (5), and low acute toxicity (0), the EH index attributed to both substances will be 11. Thus, the EH of both substances is equal, although they have different hazard classifications for the parameters assessed. Substances that have low acute toxicity, but are not readily biodegradable (e.g., mineral oil), may be persistent in the environment and increase the probability of causing adverse effects on aquatic organisms in long-term exposure, whereas the high potential of bioaccumulation increases the risks of chronic effects and biomagnification. On the other hand, substances that are rapidly biodegradable but are highly toxic (e.g., Ethylhexyl methoxycinnamate) can cause toxic effects on aquatic organisms. Thus, none of these parameters is more or less important than the other, and their equity of importance was considered the most environmentally protective decision to be applied in the IARA matrix.

Chemical substances can cause a variety of toxic effects on aquatic organisms. Mortality is the most common effect evaluated and required at a regulatory stage; however, other types of effects on aquatic organisms, such as endocrine-disrupting effects, may have serious ecological consequences for aquatic ecosystems (Hutchinson et al., 2000; Windsor et al., 2018). Endocrine-disrupting evaluations almost exclusively use adult fish (in vivo). However, the cosmetic industry is subject to regulation and policy regarding banning animal use for testing cosmetics; thus, the IARA matrix uses only existing data to score the cosmetic ingredients and alternative methods to animal testing (i.e., exclusively replacement). Thus, considering other adverse effects in the IARA matrix represents a challenge because of the lack of existing data and the availability of nonanimal assays to assess these specific endpoints.

The results generated by the IARA matrix also provide information for selecting the least hazardous cosmetic ingredients for developing eco-friendly cosmetic products. For instance, a product designer that aims to develop a greener sunscreen can select the safest UV filter for the aquatic environment by uploading the environmental data of a selected list of UV filters into the IARA matrix, which will quantitatively determine the EH (EH index) of the UV filter candidates, classifying them from small to great aquatic hazards. Using this scoring list, the product designer can select the UV filter with the lowest EH index. The EH index value can help verify the ecological improvement in the product formulation by determining the FI, which considers the EH index value and amount (percentage) of the cosmetic ingredient used in a formulation. Product formulas with different percentages of a cosmetic ingredient or differing in the composition of one or more ingredients may have different EH, and the IARA matrix helps identify the product formulation that presents the best environmental benefit. This approach has been used in our group to assess

TABLE 6 Comparison of two shampoo formulations for the aquatic hazard assessment

Ingredients	Formula A (%)	Formula B (%)	Active ingredient (%)	Biodegradation	Bioaccumulation	Acute aquatic toxicity	EH index	Formula A II	Formula B II
Cocamidopropyl betaine	1.0	0	50	0	0	4	4	0.02	-
Cocamide DIPA	0	1.0	50	4	0	5	9	-	0.045
Aqua	64.5	64.5	100	0	0	0	0	0	0
Disodium laureth sulfosuccinate	0	20.0	70	2	0	5	7	-	0.980
Sodium laureth sulfate	20.0	0	70	1	0	3	4	0.560	-
Phenoxyethanol	0.5	0.5	100	1	0	0	1	0.005	0.005
Acrylates copolymer	8.0	8.0	100	6	0	1	7	0.560	0.560
Polyquaternium-7	1.0	1.0	100	6	0	6	12	0.120	0.120
Glycerin	5.0	0	100	0	0	0	0	0	-
Dimethicone	0	5.0	100	6	6	1	13	0	0.650
								FI = 1.265 (46% more eco-friendly)	FI = 2.360

Abbreviations: EH, environmental hazard; FI, formula index determined by $\sum_{i=1}^{n} II_i$; II, ingredient index; -, no calculation because of the absence of the ingredient in the formulation.

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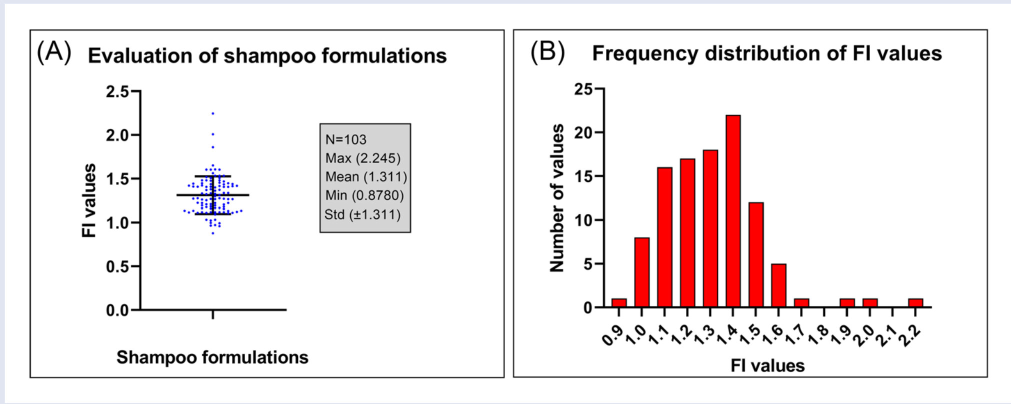

FIGURE 1 Evaluation of different shampoo formulations to reduce their aquatic hazard. (A) Each dot represents a single formula index (FI) value of a shampoo formulation. Bars represent the mean, and standard deviation of the 103 formulations evaluated. (B) The bars represent the number of FI values for each FI obtained after aquatic hazard assessment by the IARA matrix

103 different shampoo formulations in which descriptive statistics were applied to their FI data. The mean, standard deviation, maximum and minimum values, and frequency distribution of FI allowed a general overview of the EH assessed for the different formulations. Minimum or mean FI values can be used as thresholds for future formulations as a strategy for reducing the EH of a cosmetic product (Figure 1). Thus, apart from scoring the EH of cosmetic ingredients, the IARA matrix supports achieving greener cosmetics by quantitatively determining the gain in reducing the aquatic hazard of cosmetic products.

Applicability of the IARA matrix in assessing the EH of cosmetic ingredients and developing eco-friendly products

Forty-one cosmetic ingredients commonly used in rinse-off products and sunscreens were analyzed by the IARA matrix because of the relevance of these product categories to aquatic contamination. However, it is important to emphasize that the IARA matrix was not developed exclusively to assess ingredients from rinse-off products and sunscreens. It is capable of evaluating the aquatic hazard of the ingredients of many other product categories, such as fragrances and raw materials from aerosols.

The IARA assessment revealed the highest EH indexes for the UV filters butyl methoxydibenzoylmethane, ethylhexyl methoxycinnamate, homosalate, and octocrylene, and classified them among the top 10 hazardous cosmetic ingredients. This result agrees with current concerns about the impacts of sunscreens on aquatic environments (Danovaro et al., 2008; Raffa et al., 2019; Yuan et al., 2022).

Among the seven UV filters evaluated, butyl methoxydibenzoylmethane, ethylhexyl methoxycinnamate, and octocrylene are the most used in PCPs, and their average amount in PCPs is estimated as 2.6%, 4%, and 6%, respectively (Manová et al., 2013). Ultraviolet filters can reach the aquatic environments through effluent discharges or release from the skin during sports or recreation activities (Giokas et al., 2007). A maximal release of 966 kg of UV filter per year in small lakes of Switzerland was estimated assuming a maximum concentration of daily use of 1.263 mg UV filter per person (Brausch & Rand, 2011); however, precise information on the environmental concentrations of UV filters is limited because of the lack of analytical methods (Giokas et al., 2007).

Regarding bioaccumulation potential, except for the inorganic UV filter titanium dioxide, all the UV filters evaluated by the IARA were classified in moderate to high bioaccumulation categories, with scores ranging from 2 to 4. According to the scientific literature, organic UV filters are proven to be bioaccumulative (Lozano et al., 2020). Organic UV filters are highly hydrophobic (high log K_{ow}), resulting in bioaccumulation in aquatic species (e.g., crustaceans, mollusks, fish, and mammals; Lozano et al., 2020), and the bioconcentration varies among species, being higher in species with a high body content of lipids (Gago-Ferrero et al., 2015; Sancho et al., 1997). Although biomagnification has been poorly documented, fish species at higher trophic positions presented higher concentrations of UV filters than small fish (at lower trophic positions), suggesting the occurrence of biomagnification (Lozano et al., 2020). Octocrylene, one of the most lipophilic assessed UV filters classified by the IARA in category 4 for bioaccumulation, is the most frequently found UV filter in fish of some rivers of Spain (Iberian rivers; Gago-Ferrero et al., 2015). In fact, bioaccumulation and evidence of trophic magnification in fish from Iberian river basins were already demonstrated for UV filters (Gago-Ferrero et al., 2015).

Toxic effects on aquatic organisms have also been reported for UV filters (de Silva et al., 2022), and recently, the scientific community has been concerned about the capacity of UV filters to induce endocrine-disrupting effects on aquatic organisms (Brausch & Rand, 2011; Maipas & Nicolopoulou-Stamati, 2015; Wang et al., 2016). Sobek et al. (2013) estimated that almost 50% of the UV filters approved for cosmetic products by European legislation are dangerous to aquatic environments. The IARA matrix classified four out of seven UV filters (butyl methoxydibenzoylmethane, ethylhexyl methoxycinnamate, octocrylene, and homosalate) in category 6 (very high) for acute aquatic toxicity. Titanium dioxide and ethylhexyl salicylate earned low scores (0–1) for this parameter. However, it has already been demonstrated that titanium dioxide can increase its aquatic toxicity when in a mixture with parabens (Soler de la Vega et al., 2019), demonstrating that sunscreen toxicity may also depend on the other compounds of the formulation.

Considering the potential harm of UV filters to the environment, some UV filters are currently banned in some countries or specific regions of a country; thus, banning UV filters is subject to specific legislation and is not globally accepted. The UV filters ethylhexyl methoxycinnamate (or octinoxate) and benzophenone-3 (or oxybenzone) have already been banned in Palau, US Virgin Islands, Hawaii, Bonaire, and Key West, Florida (Miller et al., 2021; Raffa et al., 2019). Octocrylene has also had its use prohibited in Palau and US Virgin Islands, whereas Aruba has only prohibited the use of benzophenone-3 (Miller et al., 2021). These regions are rich in coral reef sites, and the prohibition was specifically established to achieve reef protection (Raffa et al., 2019). Octocrylene was classified by the IARA matrix as the most hazardous UV filter for the aquatic environment; however, this does not indicate the need to ban this and other UV filters or any other ingredients classified among the top list of aquatic hazards. Their safe use in cosmetic products must be evaluated case by case, considering the amount incorporated in the final product, market, and the particularities of the commercial region.

Unlike UV filters, cosmetic ingredients in the category of conditioners/humectants were identified by the IARA matrix as the least hazardous substances for aquatic ecosystems (lowest EH indexes from 0 to 3), except *B. parkii* (shea butter) because of its high bioaccumulation potential (EH index of 5).

Shea butter is a natural fat extracted from the seed of the shea tree (*B. parkii*) using organic solvents (Kar & Mital, 1981), and the amount of its use in cosmetic products is estimated as 30% of rinse-off product formulations and 60% of leave-on product formulations (Belsito et al., 2011). However, although frequently incorporated in cosmetic products, shea butter is poorly assessed for impacts on aquatic environments, and its evaluation is restricted to toxicity endpoints for human health, which classified shea butter as a safe cosmetic ingredient (Belsito et al., 2011). We performed an assay to obtain data on the aquatic toxicity (algae) of shea butter, and the EC50 value does not indicate significant toxic potential to aquatic organisms. Thus, shea butter was classified in the category of low hazard for biodegradation and aquatic toxicity (1), but the partition coefficient test (OECD 107/1995) indicated a moderate bioaccumulation potential (score 3), increasing the EH index compared with other conditioners/humectants ingredients. Like shea butter, the emollient glycol distearate is considered as having a low concern for biodegradability and aquatic toxicity (both in the category of low hazard) but presents very high bioaccumulation potential (EH index 6). Its log K_{ow} of 8.8 indicates that this cosmetic ingredient is highly lipophilic. Nevertheless, there is no evidence of environmental bioaccumulation or toxic effects of glycol distearate; thus, this emollient does not raise a concern as other emollients, such as mineral oil and dimethicone, which presented higher EH indexes (11 and 13, respectively).

Dimethicone is a volatile methylsiloxane commonly known as silicon and widely used in cosmetic formulations to soften, smooth, and moisten due to its unique properties, such as high thermal stability and smooth texture (Capela et al., 2016; Montiel et al., 2019). The high EH index of 13 obtained for this ingredient agrees with the recent concerns about silicones. In fact, silicones are not readily biodegradable (6) and have high bioaccumulative potential (6), increasing the risk of adverse effects on humans and the environment impacts (He et al., 2003; Johnson et al., 2011; Quinn et al., 2007). Thus, it is highly recommended to be replaced with less harmful ingredients (Montiel et al., 2019).

Paraffinum liquidum (mineral oil) is commonly used in cosmetic products because it is an excellent moisturizer and emollient and provides a lipophilic base to deliver active ingredients (Concin et al., 2011). Formulas for creams and lotions, bath oils, lipsticks and lip glosses, sun creams, and hair products often contain mineral oils (Concin et al., 2011). The IARA matrix predicted a high EH for mineral oil (EH index of 11) because of its high bioaccumulation potential (5) and very low biodegradability (6). For acute aquatic toxicity, mineral oil received a score of 0 and was classified as low hazard. The bioaccumulation potential and low biodegradability of mineral oil are reported extensively in the scientific literature (Barp et al., 2017; Concin et al., 2011; Cravedi et al., 2017; Nygaard et al., 2019), corroborating the IARA prediction. The low biodegradability increases the bioavailability of mineral oil to aquatic species and may result in long-term toxicity. Chronic exposition of sea scallops (*Placopecten magellanicus*) to mineral oil increased mortality and caused reproductive and developmental harm (Cranford & Gordon, 1991). Thus, although mineral oil was in the category of low hazard to aquatic toxicity, the chronic toxicity found in the literature draws attention to the need for further investigation of its toxicity in long-term exposure.

Preservatives are used in cosmetic products to prevent microorganism growth, increasing their stability. Among the preservatives evaluated, only triclosan raised high concerns related to EH; this prediction agrees with the scientific literature. Aldehydes, alcohols, and acids are readily biodegradable and generally present low to moderate toxicity for aquatic organisms (LC50/EC50 10–100 mg/L; Tolls et al., 2009). Triclosan (EH index of 14) has its use restricted in cosmetics because of safety concerns for human health (Shrestha et al., 2020; Weatherly & Gosse, 2017) as well as to the environment (Olaniyan et al., 2016; Tatarazako et al., 2004; Yueh & Tukey, 2016).

Surfactants are classified as nonionic, anionic, and cationic, and they have several applications in cosmetics, such as cleansing, foaming, and emulsifying effects, among other factors (Cowan-Ellsberry et al., 2014). In general, anionic

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surfactants do not pose a risk to aquatic ecosystems (Cowan-Ellsberry et al., 2014). In this study, the anionic surfactants sodium laureth sulfate, sodium laureth sulfate/disodium laureth sulfosuccinate, and sodium lauryl sulfate had an EH index of 4, and they do not raise concerns related to impacts on aquatic environments caused by their rapid biodegradation and low potential for bioaccumulation. Cocamidopropyl betaine is an amphoteric surfactant (i.e., both anionic and cationic structures are found in one molecule) and present low EH because of its fast biodegradability, which has been reported in a scientific study (Sun et al., 2004). In contrast, the surfactants cetrimonium chloride and cocomida DIPA yield EH indexes of 13 and 9, respectively, thus presenting considerable concern about EH. Cetrimonium chloride—a preservative, surfactant, and antistatic—is persistent (a very low biodegradability of 6) and has a very high acute aquatic toxicity (6). A report by the Danish Environmental Protection Agency (DEPA) stated that cetrimonium chloride threatened aquatic environments through its high acute toxicity (LC50 of 0.19 mg/L in fish; DEPA, 2015).

Conditioners that function as pH regulators (e.g., glycerin, sorbitol, propylene glycol) and panthenol received scores of 0, indicating that they do not raise concerns for aquatic ecosystems. For instance, glycerin has been considered a renewable cosmetic ingredient in the lubricant market, replacing mineral oil in hydraulic fluids, reducing the environmental impacts related to its use (D'Avino et al., 2015). The glycerin evaluated here is derived from vegetable oils; however, glycerin can have other sources, petrochemical or animal, and thus can have different implications for the process of product sustainability because it would decrease the proportion of renewable ingredients (Quispe et al., 2013).

In fact, the comparison of the two shampoo formulations presented in this study demonstrated that replacing hazardous ingredients in a cosmetic product formulation can effectively reduce the EH of a product, contributing to the development of eco-friendly products. The emollient dimethicone (EH index 13) was replaced by the conditioner glycerin (EH index 0) in formula A, and the surfactants contained in formula B (cocamide DIPA and disodium laureth sulfosuccinate, EH index of 9 and 7, respectively) were replaced by sodium laureth sulfate (EH index 4) in formula A, which predicts 46% less aquatic hazard for formula A, compared with formula B. Also, a less hazardous cosmetic product can be achieved by changing the amount of the ingredients in the formulation, and the determination of FI helps identify the best formula candidate for an eco-friendly product.

Although not evaluated in this study, other cosmetic categories such as dyes and fragrances are also applied in a wide variety of PCPs (e.g., hair dyes, perfumes, moisturizers, and other cosmetics) and can harm aquatic life (Bilal et al., 2020; Maiti et al., 2020; Salvito et al., 2002), indicating the importance of the hazard assessment of these other cosmetic categories, which can also be evaluated in the IARA matrix. We hope that this integrated strategy helps mitigate the EH of cosmetic products.

The development of this tool does not have commercial purposes. By publishing the IARA matrix, we aim to help researchers and R&D formulators at global cosmetic companies choose better options to formulate less hazardous products for the aquatic environment by using the data of the ingredients available herein or by following this model to create their own analytical tool.

CONCLUSION

This study described a novel EH scoring system, the IARA matrix, and demonstrated its applicability in assessing the aquatic hazard of cosmetic ingredients from available data or data from nonanimal tests. The EH indexes of cosmetic ingredients from rinse-off and sunscreen products obtained by the IARA in an integrated strategy approach to environmental data (bioaccumulation, biodegradation, and acute aquatic toxicity) agreed strongly with current environmental contamination concerns reported in the literature. The contribution of this scoring tool in selecting safer ingredients and product formulation with no or low EH contributing to product sustainability was also achieved and demonstrated in this study. However, although the IARA could correctly predict the aquatic hazard of cosmetic ingredients, the limitation in applying this tool lies in the scarcity of some environmental data, and in vitro methods seem to promise to fill this gap. In summary, the hazard assessment approach proposed here can drive safer cosmetic products to the aquatic environment, framing them in an eco-friendly context.

AUTHOR CONTRIBUTION

Natália de Albuquerque Vita: Validation; visualization; writing—review and editing. **Irisdoris Rodrigues de Souza**: Validation; visualization; writing—original draft; writing—review and editing. **Andrezza Di Pietro Micali Canavez**: Validation; visualization; writing—review and editing. **Carla A. Brohem**: Validation. **Dâmaris Marios Ferreira Pinto**: Validation; visualization; writing—review and editing. **Desirée Cigaran Schuck**: Validation. **Daniela M. Leme**: Validation; visualization; writing—review and editing. **Márcio Lorencini**: Validation.

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CONFLICT OF INTEREST

The authors declare no conflicts of interest.

DISCLAIMER

The cosmetic ingredients assessed in this case study do not necessarily reflect the ingredients applied in the cosmetic products of the Grupo Boticário.

DATA AVAILABILITY STATEMENT

Data, associated metadata, and calculation tools are available from corresponding author Andrezza Di Pietro Micali Canavez (andrezza@grupoboticario.com.br).

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SUPPORTING INFORMATION

Table S1: Websites of databases and governmental and accreditation bodies.

Table S2: Summary of the hazard classification described in EPA, C2C, and the European Regulation 1272/2008 for biodegradation, bioaccumulation, and acute aquatic toxicity. Representing the most conservative classification values chosen to be applied in the IARA matrix.

Table S3: Collected data on bioaccumulation, biodegradation, and acute aquatic toxicity of cosmetic ingredients from rinse-off products.

Table S4: List of the two different shampoo formulations used to exemplify the use of the formula index (FI).

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