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Characterizing and quantifying chemical ingredient use in consumer products between two separate databases and implications for environmental and human health exposure

Todd Gouin

Research Consulting, TG Environmental Research, Bedfordshire MK44 1PL, UK.

Correspondence to: Dr. Todd Gouin, Research Consulting, TG Environmental Research, 18 Wellpond Close, Sharnbrook, Bedfordshire MK44 1PL, UK. E-mail: todd.gouin@environresearch.com

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Abstract
Assessing chemical exposure in home and personal care products (HPCPs) represents an important data need. Key challenges to the assessment are related to limited knowledge in quantifying and characterizing the weight-fraction inclusion level and functionality of chemicals in HPCPs. Publicly available tools have been developed to address these challenges, such as the Chemical and Products database (CPDat). This study aims to evaluate the relative performance of CPDat by comparing estimates of weight-fraction inclusion level and functionality to other relevant data sources. Specifically, estimates obtained from CPDat are evaluated and compared with estimates obtained from marketing analytic data, using Euromonitor Passport for 31 commonly used chemicals found in HPCPs. The results obtained from this exercise suggest relatively good agreement between each of the methods for 10 chemicals (ρ = 0.92; *P*-value =0.02). When considering all 31 chemical ingredients, however, the correlation observed is generally poor (ρ = 0.46; *P*-value = 0.1), which is attributed to differences in how the underlying data are obtained for each method. With an emphasis on obtaining data based on mining datasheets for individual products, the application of CPDat is suggested to be useful for higher tiers of assessment, with data obtained from marketing analytics providing valuable input to exposure-based screening models. The insight gained from this study can be used to help guide the appropriate use of data obtained from different sources within a tiered exposure assessment.

Keywords: Exposure, household and personal care products, chemical and products database, Euromonitor

INTRODUCTION

Estimating the exposure to support the environmental and human health risk assessment of chemicals used in commerce is typically based on one of two methods. The first approach is to obtain manufacturing data of annual tonnages of the chemical ingredient for a specific geographic region, as might be obtained directly from chemical manufacturing companies. This gives a crude estimate of consumer exposure, whereby chemical ingredients are assumed to be widely dispersed, with an assumption that the chemical is used by many users and that there exists the potential for both human and environmental exposure. A second approach, representing a higher level of refinement, is to estimate consumer exposure to chemicals used in specific downstream consumer products that may contain the chemical, and for which a maximum weight-fraction inclusion level and a high percentile value (such as 90th or 95th) for the amount of product used by consumers for each application are assumed. The individual, high-end exposures are then simply summed to give an aggregate exposure, which also results in a conservative exposure estimate. A key challenge, however, regards the characterization and quantification of how chemicals are used in downstream consumer products, whereby significant variability related to the use of a chemical exists.

Recently, there have been various attempts to develop methods to incorporate information on non-use and co-use of products to derive a more accurate estimate of aggregate exposure. For instance, Cowan-Ellsberry and Robison[1] used a limited data set of consumer habits coupled with maximum inclusion levels of parabens to demonstrate how the variance in consumer behavior can significantly influence the exposure estimate compared to one based on using simple addition methods. Similarly, Gouin *et al.* demonstrated how differences between the use of D5 in products with a "leave-on" use scenario versus products, such as shampoos, representative of a "down-the-drain" use scenario, significantly influence the environmental exposure and overall fate of the chemical[2].

Advances in methods to refine estimates of exposure that utilize consumer use and habit data, as well as marketing and economic indicators, have been demonstrated in several studies[3-11]. The studies cited are illustrative of the various attempts to incorporate non-traditional data sources toward refining estimates of exposure. A key starting point in relation to the use of chemicals in downstream products, such as household and personal care products (HPCPs), is related to the applied dose, which in this instance, is characterized by the amount of chemical that might be present in a product represented as a weight-fraction inclusion level, and how that product is used by the consumer[12]. Refinement of exposure, based on probabilistic approaches related to the applied dose, has been developed. For instance, studies have been conducted to assess consumer use and behavior habits about various product types[12-16], whereas total amounts that might be emitted to the environment have been estimated based on information pertaining to GDP and using sales and marketing data[5,17,18]. The information obtained from these studies characterizes the probability distributions associated with the amount of product used by consumers in various geographic regions. Additional information regarding total aggregate exposure, simulated use studies, and probabilistic distributions related to variability associated with physiological data, such as body weight, variance in skin thicknesses, etc., can also be included in refining the overall characterization of the applied dose[11]. When estimating environmental exposure, data related to the removal efficiencies of a chemical in wastewater treatment systems, such as due to biodegradation and sorption processes, and variance in hydrological processes, are needed to better predict environmental concentrations in surface waters[19].

In 2010 the U.S. EPA commissioned the National Research Council (NRC) to develop a report to advance exposure science in the 21st century[20]. The report draws attention to advances in exposure science - a key component of which identifies a framework for the collection, storage, interpretation, and application of data from various sources. The proposed framework emphasizes a holistic approach for bringing together various types of data, with the U.S. EPA taking a leadership role in the development and application of a suite of tools aimed at supporting a robust assessment of exposure[21].

The development of tools by the U.S. EPA has resulted in novel approaches that attempt to utilize chemical descriptors as a basis for estimating how chemicals might be used in consumer products[9,22-24]. These developments have resulted in the creation of the chemical and products database (CPDat)[25]. Information obtained from CPDat is thus perceived as representing a valuable source of information as input data for estimating chemical exposure, which theoretically could be used to help inform both the human and environmental risk assessment of chemicals used in commerce.

A key challenge, however, relates to obtaining realistic data on product co-use, chemical concentration and chemical occurrence in HPCP formulations. One method developed by the US EPA has been to estimate both the functional use of a chemical within a product and its weight fraction through the application of a Quantitative Structure Use Relationship (QSUR)[25]. The QSUR, based on information obtained from various publicly available data sources, such as information obtained in Material Safety Data Sheets (MSDS) and accessing information from various other online resources, promises to represent a potentially valuable resource for estimating exposure concentrations of chemicals used in HPCPs. Efforts to evaluate the relative performance and reliability of the information used in developing CPDat would thus help strengthen the broader application of the tool.

As an alternative approach to obtaining exposure data, it may be useful to consider the application of proprietary information available through various market survey databases, such as those provided by Mintel, Kantar Worldpanel, and Euromonitor International, which have recently been used to provide novel sources of data for helping to support chemical exposure assessment[5-8]. This is because they can be used to refine exposure parameters, i.e., chemical concentration data used in products and specific market regions, based on their surveys of market sales data, consumer purchasing habits, and innovations in HPCP formulation design and product claims.

Proprietary databases, such as those available through Euromonitor International, which describes itself as the world's leading independent provider of global strategic intelligence on industries, countries, and consumers, may provide a novel approach to assessing exposure based on marketing analytics. The marketing analytics data included in the Euromonitor International Passport database - an online proprietary searchable tool that provides clients with access to information specific to their needs - enables trends with respect to both temporal and spatial scales, from global to regional to national, to be evaluated with respect to consumer products available within specific markets. Information includes details of companies and brands sold in different countries and summarize the data in terms of sales, which can be further converted to tonnage volumes of product categories sold.

Furthermore, within each product category, information for companies and brands sold within a market over a specified timeframe is monitored and can be extracted into Excel spreadsheets for further analysis. Information for each product type can then be extracted in terms of total volumes sold to a geographic market. In addition to providing volumes of a product category sold in a business market, Euromonitor Passport also monitors trends in chemical ingredients used in different product categories as well as information on weight-fraction inclusion levels.

The Euromonitor Passport software thus provides the opportunity to access high-level information related to the use of chemical ingredients within specific markets and consequently represents significant potential for use in assessing the relative performance of public tools, such as the US EPA CPDat. In this study, weight fraction inclusion levels and functional use data derived from the Euromonitor Passport database are thus used to compare against weight fraction inclusion levels and function use data derived from US EPA CPDat. Ideally, knowledge pertaining to both the weight fraction inclusion levels of a chemical ingredient, along with its functional use in a product category, can help inform estimates of exposure for chemical ingredients used HPCPs. Lastly, the strengths and weaknesses of each of the approaches are evaluated, based on an analysis of a subset of chemical ingredients found in HPCPs for the USA market between 2018-2019.

EXPERIMENTAL

To compare the output between the US EPA CPDat and data extrapolated from the Euromonitor Passport database, more than 70 individual chemicals and chemical ingredient mixtures and characteristic of those used in HPCPs, and representative of various functionalities and uses in a broad range of HPCPs were identified [Supplementary Materials 1]. The selection of the chemicals was further informed based on the availability of complementary data reporting their use in various HPCPs, obtained from summary reviews regularly published by the Cosmetic Ingredient Review (CIR) (https://www.cir-safety.org/). Information summarizing the range of inclusion levels and functionality as published by the CIR is presented in Supplementary Materials 2. Taking into consideration the information obtained from the CIR and to enable a robust analysis between CPDat and data extrapolated from the Euromonitor Passport database, the CAS numbers of 31 individual chemical ingredients, representative of primary chemicals typically associated with the various ingredient groupings used in HPCPs, were selected as the primary focus for data analysis and interpretation.

The most recent version of CPDat (Wall *et al.*, 2020) was used to obtain information on the use of chemical ingredients in HPCPs. The data included in this version represents an update to the information in the 2018 release[25], which includes new data curation and management system features, referred to as Factotum, developed to increase the volume and reliability of the data available for chemical use in HPCPs. The data release contains additional machine-readable data and data associated with the latest curation activities. The consumer products included in CPDat for exposure assessment and modeling have been primarily curated manually into product use categories[26]. The chemical ingredients identified in individual products are assigned a chemical record ID, associated with a reported chemical name and CAS number, if available. Each individual chemical ingredient record is then curated based on automated workflows within the US EPA's Distributed Structure-Searchable Toxicity (DSSTox) database[27], where they are assigned a preferred name, CAS, and a DSSTox chemical Substance ID (DTXSID). Chemical records not yet officially curated into DSSTox (i.e., awaiting formal curation) are assigned a provisional preferred identifier and DTXSID based on the official curation of other CPDat records with identical reported identifiers. Thus, the CAS numbers for each of the 31 chemical ingredients were used as the primary input for identifying chemicals within CPDat in product use categories consistent with personal care and cleaning/household care products[26] (i.e., identified as being most representative of HPCPs). In some instances, however, chemical ingredients may contain > 1 CAS number, in which case, each CAS number was used to extrapolate data from CPDat and a manual check of the DTXSID was performed to ensure consistency. In instances where products identified in CPDat contain information for a chemical ingredient without listing its CAS number, the DTXSID was used to ensure that all products reporting the use of each of the 31 chemical ingredients were adequately captured.

Euromonitor Passport lists ingredients used in HPCPs either as part of an ingredient grouping or as a specific chemical ingredient. Over 450 chemical ingredients and ingredient groupings are individually defined [Supplementary Materials 3]. Data related to the use of chemical ingredients extrapolated from the Euromonitor Passport database were thus obtained by either aligning an individual chemical ingredient to its appropriate chemical ingredient group or using the information reported for that specific chemical ingredient, depending on how the information is presented in Euromonitor Passport. The information for chemical ingredients originating from chemical ingredient groups is obtained based on the CAS number listed for that chemical ingredient, as reported by Euromonitor Passport, and is identified as a representative chemical ingredient for the entire chemical ingredient group. Consequently, the information obtained from the definitions of chemical ingredients and ingredient groups represents an important source of data to ensure an accurate comparison between CPDat and data extrapolated from the Euromonitor Passport database.

Figures 1 and 2 summarize each of the product categories defined in the Euromonitor Passport Database for beauty and personal and home care products, respectively. The extrapolation of chemical ingredient tonnage and their breakdown between 2014-2019 for the U.S. market was obtained by accessing the online Euromonitor Passport Database dashboard for each product category illustrated in Figures 1 and 2.

The underlying data reported in Euromonitor Passport are based on sales data, whereby the number of units for a product category is used to estimate either the monetary sales number (e.g., U.S. dollars) or the volume of product sold (e.g., tonnes). The data that populate the Euromonitor Passport database are based on market research surveys used extensively by HPCP businesses to understand global and regional markets, and have been observed to be reliable compared to internal sales data[5]. The derivation of ingredient volumes is based on knowledge obtained regarding the ingredient listing of a product category, which results in product-specific recipes being developed. For instance, a product may be found to contain several ingredients as listed on the product label. Market research performed by Euromonitor results in an estimate of the percent weight fraction for each chemical ingredient. If 100 units of the product are sold in a market, with a weight of 100g/unit, then an estimate of 10kg of product is obtained. If chemical "A" represents 10% of the ingredients used in the product, the total chemical ingredient used would then be 1kg. Since data regarding the actual weight fraction percent inclusion levels of chemical ingredients used in HPCPs are proprietary, only total volumes for chemical ingredients and product categories are reported by Euromonitor Passport. Consequently, the extrapolation performed here involves estimating the weight fraction inclusion level by dividing the volume of chemical ingredient (V_x) reported for a product category by the total volume sold (V_T) (i.e., weight fraction = V_x/V_T, where both V_x and V_T are obtained directly from the Passport database). A limitation of the approach used, therefore, is an assumption that the chemical ingredient is used at a relatively consistent level across all individual products used within the product category. Chemical ingredients used in a small number of products may not be adequately captured using this approach, depending on the overall market share of the product. Finally, since the approach described here requires inputs on the use of specific chemical ingredients, the approach will be ineffective for chemicals not included in the Euromonitor Passport database.

The comparison of weight-fraction inclusion levels reported between CPDat and those extrapolated from the Euromonitor Passport database is based on evaluating similarities between the mean, median, and variance in the weight fractions obtained from each method. This information is further supplemented by data reported by CIR. Similarly, the functional use of chemical ingredients reported in CPDat is compared against the Euromonitor Passport ingredient definitions, information that is further complemented by summaries published by CIR.

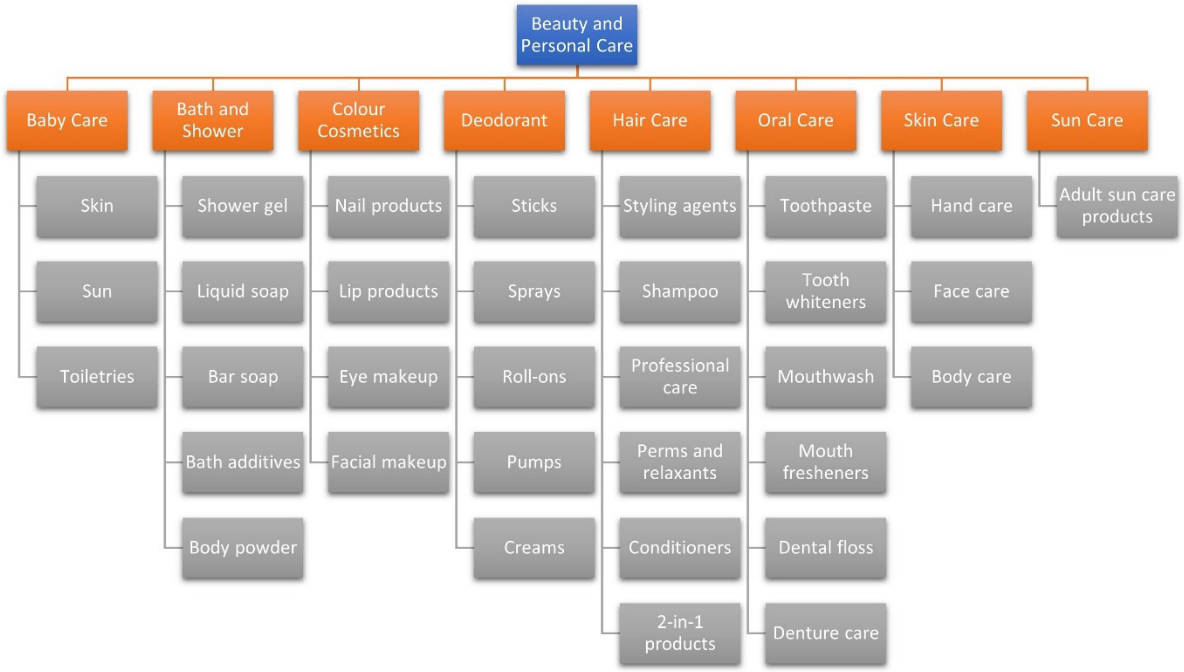

Figure 1. Summary of all product categories used in evaluating chemical ingredient weight fractions per personal care product category.

Figure 2. Summary of all product categories used in evaluating chemical ingredient weight fractions per home care product category.

RESULTS AND DISCUSSION

Data reporting the use of functional ingredients and percent inclusion levels obtained from CIR for various chemical ingredient groups and specific chemical ingredients are summarized in Supplementary Materials 2, with the properties of chemical ingredients further summarized in Supplementary Materials 1. The chemical ingredients identified for evaluating the various sources of information are observed to represent approximately 40% of total ingredient tonnage used in personal care products (≈ 8.5×10^5 tonnes/2×10^6 tonnes) and about 20% of total ingredient tonnage used in home care products (≈ 1.6×10^6 tonnes/8.7×10^6 tonnes), which is based on an evaluation of the data obtained from the Euromonitor Passport database. It is further noted that the single largest volume ingredient used in both personal and home care products is listed as aqua (i.e., water), which represents about 57% and 65% of total tonnage used in personal and home care products, respectively. The chemical ingredient categories and the specific 31 chemicals selected are thus presented as representing the most dominant uses of chemicals found in HPCPs. Given the high probability of the use of the 31 chemical ingredients in various HPCPs, it is thus reasonable to assume that an evaluation between CPDat and Euromonitor Passport for this group of chemical ingredients should provide a robust analysis for comparison purposes.

Each category documented within the Euromonitor Passport Database is segmented into sub-categories [Figures 1 and 2], information from which is used to estimate the relative ingredient weight fraction for a particular product type. Of the different product categories shown in Figure 1, bath and shower products are observed to dominate the total tonnage of ingredients used (≈ 6×10^5 tonnes), whereas laundry products represent the largest category (≈ 4×10^6 tonnes) for home care products [Figure 2]. The chemical ingredient weight fractions for 31 chemicals, representative of key ingredient categories, are summarized in Figure 3, with a side-by-side comparison between data extrapolated from CPDat and Euromonitor Passport illustrated. The correlation between the two sources of data for all 31 chemical ingredients is observed to be generally poor ($\rho = 0.46$, *P*-value = 0.1). There is, however, a subset of 10 chemical ingredients for which the correlation is good ($\rho = 0.92$, *P*-value = 0.02), which is discussed in more detail below.

Table 1 summarizes the results obtained from the CIR, CPDat, and Euromonitor Passport with respect to the functional use of each chemical ingredient and the median inclusion levels, illustrated in Figure 3. Additionally, Table 1 also reports the total number of entries reported in CPDat for each chemical ingredient and the fraction of entries that include information reporting the weight fraction inclusion level. The weight fraction inclusion levels summarized for each chemical ingredient taken from CIR represent the maximum and minimum values reported. Since the information presented in the CIR for chemical ingredients does not include sufficient details regarding the distribution of use, it is not possible to represent the data as a probability distribution in Figure 3. The details obtained from the CIR, therefore, are used to reflect the range of values reported in various product categories, which is further used to support the discussion below.

When comparing the weight fraction estimates of data extrapolated between CPDat and Euromonitor [Figure 3], various interpretations are possible. In many instances, relatively good agreement between CPDat, Euromonitor Passport, and data reported in the CIR can be illustrated, an observation that should help strengthen confidence regarding the use of any of the three methods for estimating exposure. Most notable among these are the chemical ingredients, sodium laureth sulfate, sodium laurate, stearyl alcohol, ceteareth-20, benzyl alcohol, benzalkonium chloride methypropanediol, panthenyl ethyl ether, methylparaben and permethrin, illustrated as chemical numbers 2, 5, 7, 11, 13, 21, 23, 26, 27, and 31, respectively in Figure 3. The relatively good agreement between the various methods for these 10 chemical ingredients is suggested to be related to their limited functional uses, which are also limited to use in specific groups of HPCPs. For instance, the use of permethrin to treat head lice or the use of panthenyl ethyl ether as a hair conditioning agent in shampoos. While the agreement between the median values for these 10 chemical ingredients tends to be relatively good, it should be noted that there are differences in the maximum and minimum weight fraction inclusion levels, as seen in Figure 3, which results in skewed distributions that cause significant differences between the mean values of the various methods for some chemical ingredients (see Supplementary Materials 2 for additional discussion).

Conversely, however, there are several instances that result in non-intuitive differences between each of the methods, which require more in-depth evaluation regarding potential factors that might likely influence the observed inconsistencies in weight fraction inclusion level estimates. For instance, there are examples where the number of products reporting an inclusion level for some of the 31 chemical ingredients in either CPDat or Euromonitor are observed to be insufficient for a distribution capable of producing a box-and-whisker plot. This can be illustrated when considering the results obtained for the alkyl ester, myristyl laurate used as an emollient, and the silicone polymer, caprylyl methicone. Data from CPDat for myristyl laurate (Chemical 15, Figure 3) are limited to nine products, all from the same manufacturer, with the same inclusion level of 0.12%. While this information is consistent with the ranges reported by the CIR, for which

Table 1. Summary of data downloaded for each chemical ingredient used for evaluating their weight fractions distributions reported in Figure 3

			CPdat					
Chemical ID	**Chemical ingredient**	**CIR Function definition[a]**	**Estimated use function (probability)**	**Total number of entries[b]**	**Entries with weight fraction (%total)[c]**	**Median inclusion level (%)**	**Euromonitor median inclusion level (%)**	**CIR range of inclusion levels (%)**
1	Ethyl acetate (CAS No. 141-78-6)	Solvent/Fragrance	Fragrance (0.936)	1401	32 (2.3)	28.2	3	0.000002-85
2	Sodium laureth sulfate (CAS Nos. 1335-72-4; 3088-31-1; 9004-82-4, generic; 68585-34-2, generic; 68891-38-3, generic; 91648-56-5)	Surfactant	Surfactant (0.942)	1560	104 (6.7)	7.25	2.1	0.1-50
3	Isopropyl alcohol (CAS No. 67-63-0)	Antifoaming agent/fragrance/solvent/viscositydegreasing agent	Antimicrobial (0.55); fragrance (0.294)	2222	124 (5.6)	12	3.3	0.002-100
4	Butane (CAS No. 106-97-8)	Propellant	Flavorant (0.939); fragrance (0.631) - harmonized functional use reported as fragrance	279	151 (54)	33.4	0.9	1-92
5	Sodium laurate (629-25-4)	Surfactant/cleansing agent; surfactant/emulsifying agent	Surfactant (0.995); Emulsion stabilizer (0.809); Emulsifier (0.763)	8	4 (50)	1.5	1	0.005-14
6	Ethylhexylglycerin (CAS No. 70445-33-9)	Skin-conditioning agent; deodorant agent	N/A	319	49 (15)	0.1	2.2	0.000001-8
7	Stearyl alcohol (CAS No. 112-92-5)	Emulsion stabilizer; emollient; surfactant; lubricant; antifoaming agent	Emulsion stabilizer (0.987); surfactant (0.912); lubricant (0.819)	333	24 (7.2)	1.5	0.95	0.0002-18
8	Isopropyl myristate (CAS No. 110-27-0)	Skin conditioning agent/emollient/binder; fragrance ingredient	Emollient (1.00)	640	48 (7.5)	5	0.4	0.000005-77.3
9	Dimethicone (CAS No. 141-62-8; 141-63-9; 63148-62-9; 9006-65-9; 9016-00-6; 107-52-8)	Antifoaming agent; Skin protectant; Skin-conditioning agent - occlusive; Solvent	Hair conditioner (0.901); skin conditioner (0.742); adhesion promoter (0.970)	1559	104 (6.7)	2	0.6	0.0000014-85
10	Dipropylene glycol (CAS No. 110-98-5)	Humectants; emulsifiers; plasticizers; solvents	Antimicrobial (0.461)	542	24 (4.4)	2	0.15	0.004-50
11	Ceteareth-20 (CAS No. 68439-49-6)	Nonionic surfactant/emulsifier/emollient	N/A - harmonized functional use reported as ubiquitous	471	58 (12)	0.5	0.4	0.008-11
12	Steareth-21 (CAS No. 9005-00-9)	Nonionic surfactant/emulsifying agent	N/A - harmonized functional use reported as surfactant	244	29 (12)	2.2	0.3	0.01-7

13	Benzyl alcohol (CAS No. 100-51-6)	Fragrance ingredient; preservative; solvent; viscosity decreasing agent	Fragrance (0.941); preservative (0.505)	832	22 (2.6)	0.3	0.5	0.000006-10
14	Benzophenones (CAS No. 131-56-6; 131-57-7; 4065-45-6)	Light stabilizer/sunscreen agent	UV absorber (0.993)	1295	276 (21)	4	0.3	0.000035-1.6
15	Myristyl laurate (CAS No. 22412-97-1)	Surfactant/emulsifying agent	Emollient (1.0); emulsifier (0.809); surfactant (0.669)	60	9 (15)	0.12	0.85	0.1-2
16	Stearic acid (CAS No. 57-11-4)	Fragrance ingredient; surfactant/cleansing agent; surfactant/emulsifying agent	Surfactant (0.997); emulsifier (0.927)	1248	91 (7.2)	2.2	0.35	0.00006-37.4
17	Sodium cocoate (CAS No. 61789-31-9)	Skin-conditioning agent, occlusive, emollient, and moisturizer	N/A - Harmonized functional use as surfactant	60	14 (23)	11.8	0.3	1-52
18	Glycol stearate (CAS No. 111-60-4)	Emulsifiers, dispersants, opacifiers and viscosity modifiers	Emollient (0.987); emulsifier (0.941)	206	15 (7.3)	1.5	0.2	0.0001-6
19	Glyceryl stearate (CAS No. 11099-07-3 ; 123-94-4; 31566-31-1)	Fragrance ingredient; Skin conditioning agent/emollient; surfactant/emulsifying agent	N/A - Harmonized functional use as surfactant	543	47 (8.7)	3	0.4	0.0002-18.9
20	Octocrylene (6197-30-4)	Sunscreen agent	UV absorber (0.939)	410	175 (43)	3.4	1.05	Maximum = 10
21	Benzalkonium chloride (CAS No. 8001-54-5)	Foaming and cleansing agent; conditioner; bactericide	N/A - Harmonized functional use as antimicrobial	172	49 (28)	0.13	0.5	0.01-0.5
22	Caprylyl methicone (CAS No. 17955-88-3)	Skin conditioning agent - occlusive	Wetting agent (0.954); Skin conditioner (0.653); Harmonized functional use as skin conditioner	20	0 (0)	0-10	0.75	0.075-16
23	Methylpropanediol (CAS No. 2163-42-0)	Solvent	Crosslinker (0.566)	37	10 (27)	0.9	0.25	0.025-21.2
24	Polyquaterniums (CAS No. 112-03-8; 57-09-0; 112-02-7)	Film formers; hair fixatives; skin-conditioning agents-miscellaneous	N/A - Harmonized functional use as film forming agent	454	30 (6.6)	1.2	0.1	0.0008-10
25	Zinc pyrithione (CAS No. 13463-41-7)	Anti-dandruff active ingredient	N/A - Harmonized functional use as ubiquitous	94	36 (38)	1	0.2	0.5-2
26	Panthenyl ethyl ether (CAS No. 667-83-4)	Hair conditioning agent	N/A - Harmonized functional use as hair conditioner	359	88 (25)	0.1	0.6	0.001-2
27	Methylparaben (CAS No. 99-76-3)	Fragrance ingredient; preservative	Preservative (0.988); fragrance (0.567)	962	93 (9.7)	0.12	0.2	0.000001-0.9
28	Sodium lactate (CAS No. 72-17-3)	Buffering agent; skin-conditioning/humectant	Buffer (0.995)	85	5 (5.9)	10.5	0.1	0.0002-8
29	Methylisothiazolinone (CAS No. 2682-20-4)	Preservative	Antimicrobial (0.899)	724	373 (52)	0.01	0.2	0.000000035-0.01
30	Butylated hydroxytoluene (CAS No.	Preservative/antioxidant	Antioxidant (0.992);	2220	79 (3.6)	0.05	0.1	0.0002-0.5

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	128-37-0)		preservative (0.571)					
31	Permethrin (CAS No. 52645-53-1)	Insecticide	Antimicrobial (0.817)	4	4 (100)	0.56	0.1	0.5-5

[a]Based on information obtained from CIR summaries, Supplementary Information.

[b]Total number of products reported in CPDat for which chemical ingredient is included, based on information obtained from material and safety datasheets.

[c]Total number of products reported in CPDat for which a weight-fraction inclusion level is reported, based on information obtained from material and safety datasheets. N/A: No data available.

a range of inclusion levels of between 0.1%-2% is reported, it is insufficient to provide a robust evaluation of the distribution of weight fractions across different types of products. Data from Euromonitor Passport, on the other hand, are extrapolated to observe weight fractions of between 0.1%-3.9%, which is also observed to be generally consistent with the range of data reported by the CIR [Supplementary Materials 2]. In the instance of caprylyl methicone (Chemical 22, Figure 3), data obtained from CPDat are limited to two individual products, where a range of between 0%-10% is reported, which can be seen to be in good agreement with the range of data reported by CIR [Supplementary Materials 2] of between 0.075%-16%. However, because a distribution of weight fraction inclusion levels based on two individual products is not possible, there is no box-and-whisker plot for this chemical ingredient illustrated in Figure 3. Data extrapolated from Euromonitor Passport, on the other hand, results in a range of between 0.2%-1.7%, limited to the lower range of values reported in the CIR. The differences between how each of the three approaches is used to extrapolate a weight fraction inclusion level for a chemical ingredient is therefore important to consider, as there may be inconsistencies regarding the underlying data used in extrapolating the values obtained, which could result in non-intuitive differences when comparing against the various methods.

Furthermore, when considering the differences with respect to weight fraction inclusion level for each chemical ingredient, it is worth noting that some chemical ingredients may have significant differences with respect to the inclusion level depending on the type of product. For instance, the chemical ingredient category of solvents, represented by ethyl acetate (Chemical 1 in Figure 3), is shown to have significant variability depending on the product category. In nail care products, the inclusion of solvents, such as ethyl acetate, is estimated to be > 80% [Supplementary Materials 2], but in the majority of other product categories where solvents are used, inclusion levels are typically < 5% [Supplementary Materials 2]. Observations obtained from CPDat, where ethyl acetate is reported to have a maximum inclusion level of 86%, are consistent with the CIR, with nail care product categories dominating the higher inclusion levels. A notable difference, however, between the distributions in data extrapolated from Euromonitor Passport and CPDat can be seen for ethyl acetate, whereby the inclusion of products other than nail care products using ethyl acetate is possibly better reflected in the Euromonitor Passport database than it is in CPDat. The difference between Euromonitor and CPDat, therefore, relies on scrutinizing the actual products for which CPDat reports inclusion levels and evaluating if the products adequately capture the range of products in which the chemical ingredient might be used. Since the information in CPDat has been populated largely based on MSDS information, relying on the extrapolation of data from a limited number of MSDS that actually include weight fraction inclusion levels, there is the potential for some products to be missed, due to the lack of information reported in the MSDS or a lack of any available information for that product category.

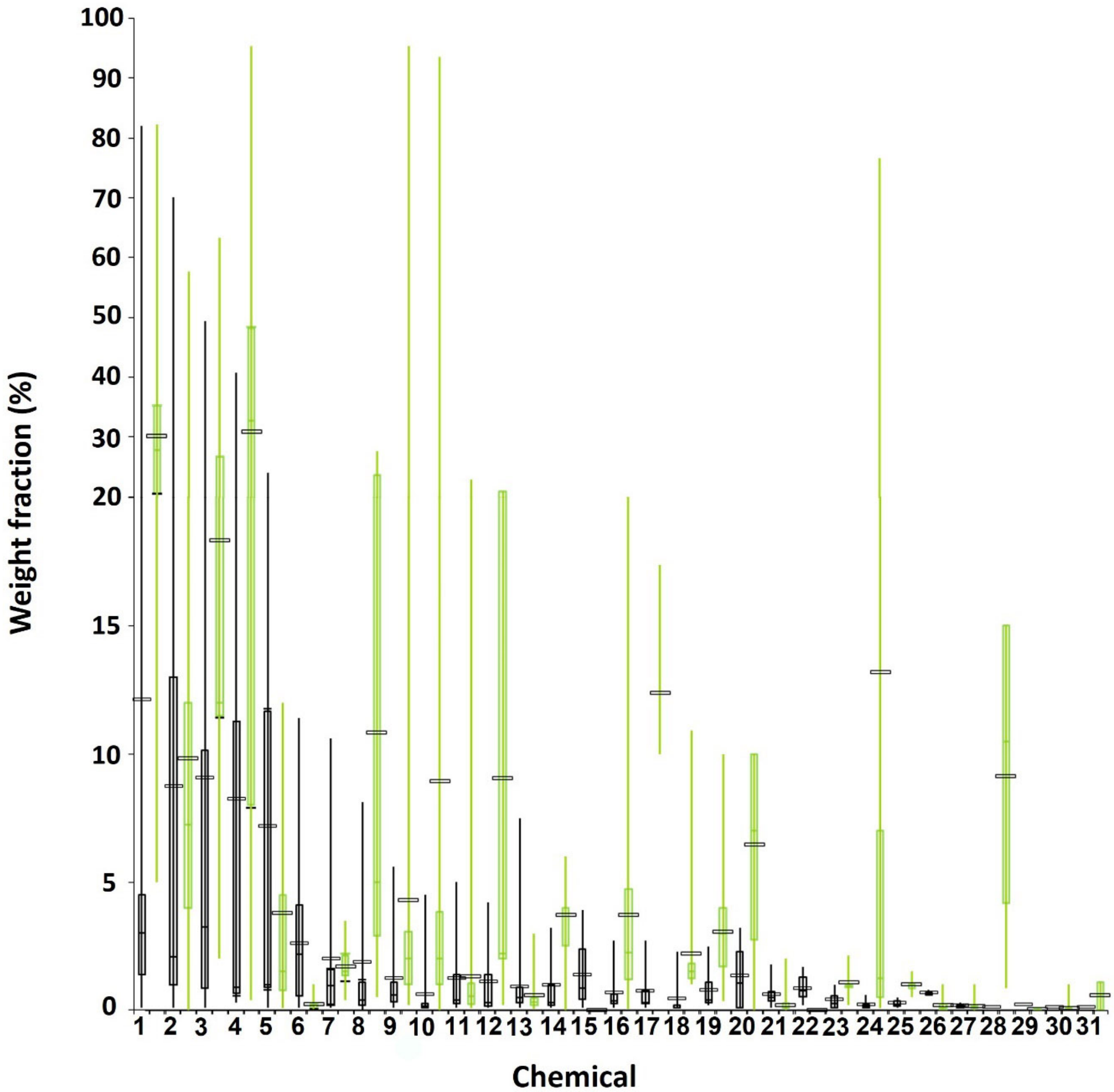

Figure 3. Box and whisker plots summarizing the distribution of weight fractions for chemical ingredients in various personal and home care product categories obtained from Euromonitor Passport (black) and CPDat (green). In the box plots, the lower box indicates the 25th percentile, the line separating the upper and lower boxes indicates the mean, and the upper box indicates the 75th percentile. The small black rectangular box represents the median value, and the whiskers above and below the box indicate the maximum and minimum values, respectively. Please refer to Table 1 for chemical names.

Table 1 summarizes the total number of individual products reporting the use of a specific chemical ingredient and the number of products for which weight fraction inclusion level data are reported. It can be seen that the use of chemical ingredients included in this assessment is highly variable, whereby depending on the chemical ingredient, the total number of products reporting its use can range from > 2000 to < 5. The evaluation, therefore, includes a combination of widely used chemical ingredients and those limited to a niche number of products. However, not all products included in CPDat report a weight fraction inclusion level, with a general observation that typically < 50% of the total number of products include this level of information. Consequently, it is important to be aware that the extrapolation of a weight fraction inclusion level from CPdat is entirely influenced by the level of information used to obtain the underlying statistics.

Similar challenges also accompany the extrapolation of data from Euromonitor Passport, whereby underlying assumptions related to the use of a chemical ingredient in a product category relative to the total tonnage use of that product category can limit the accuracy of the extrapolated weight fraction. A difference, however, between CPDat and Euromonitor Passport, is that the data used in populating the Euromonitor Passport Database are based on a combination of bottom-up and top-down extrapolation and curation methods. The bottom-up approach used in Euromonitor Passport is based on the product volumes and market share of the product brands for individual product categories sold within a specific market and used within a calendar year. This information is developed based on a review of the ingredients listed on product labels sold within a geographic market for the top brands and which is used to create individual product formulation recipes. The data produced using the bottom-up approach is then assessed for consistency by applying a top-down curation of the information, which involves a number of manual resource-intensive activities aimed at cross-validating the data through discussions with key members representing the industry, including chemical ingredient manufacturers, HPCP brand companies and trade associations. Differences can therefore be expected, between commonly used chemical ingredients associated with a product category, where it is likely that the results will provide a relatively good estimate of the weight fraction used, versus less commonly used chemical ingredients.

An important factor influencing the variability in the weight fraction inclusion level, as reported in the summary reviews by CIR [Supplementary Materials 2] and the ingredient definitions obtained from Euromonitor Passport [Supplementary Materials 3], is the influence of the various functionalities for which certain chemical ingredients are used. In addition to extrapolating information on the weight fraction of chemical ingredients, CPdat also includes the capability for estimating the functional use of a chemical based on output obtained from a QSUR[10]. Table 1 includes the probability output for the estimated functional use of each chemical ingredient as obtained from CPdat, and in some instances where a probability was not possible, the reported harmonized functional use. Generally, the agreement between CPDat pertaining to functional use and information summarized from CIR is seen to be relatively good. However, there are several instances where the agreement is poor or for which an estimated use is not reported. In some instances, such as for sodium cocoate, steareth-21, and the polyquaterniums, where no functional use estimate is reported, the harmonized functional use listed is in good agreement with the CIR for those chemical ingredients. On other occasions, such as for zinc pyrithione and ceteareth-20, the harmonized functional use is listed as ubiquitous, although the reported functional uses are consistent with the CIR. Consequently, users of the QSUR will need to apply their own best judgment regarding the functional use of these chemical ingredients, which in these instances could result in ambiguity. Finally, dipropylene glycol, butane, and methylpropanediol have estimated functional uses that are simply inconsistent with the summary information reported in CIR. A key challenge, therefore, when relying entirely on the QSUR to obtain information on the functional use of a chemical ingredient to potentially align with a weight fraction inclusion level, relates to how to best address the ambiguity and inconsistency between the information presented in CPDat and the actual reported use, harmonized functional use and the estimated functional use.

When considering the application of CPDat and/or the Euromonitor Passport database as resources for informing the exposure assessment for chemical ingredients used in HPCPs, it is important to consider each approach's relative strengths and weaknesses. A strength of the Euromonitor Passport Database is the capability to obtain annual tonnage data for individual product categories for a specific geographic market. Given the resource invested annually for populating the underlying data that inform the tonnage values reported in the Passport database, it is possible to monitor and screen potential changes in chemical ingredients on a year-by-year basis. For instance, the recent issue of microplastic in the marine environment resulted in all major consumer product companies voluntarily phasing out the use of polyethylene microbeads as an exfoliant in their HPCPs, which was further supported by regulatory activity aimed at banning their use in rinse-off products[6]. The use of polyethylene beads as an abrasive in bath and shower products reported in Euromonitor accurately captures these actions, whereby the annual use of polyethylene in these products in the U.S. declines from > 150 tonnes in 2014 to zero after 2016. Increases in other types of materials that might be used as an exfoliant in bath and shower products can be seen after this period, such as silica, nut shells, and crushed seeds, which presumably reflect the adoption of alternative materials aimed at replacing polyethylene microbeads as exfoliant agents.

In CPDat, there are 450 individual products listing polyethylene as an ingredient, with 10 products reporting weight fraction inclusion levels ranging from 0.4%-83%. The highest inclusion (83%) is listed for a cosmetic make-up product. The median inclusion level is 4.5%, with uses in rinse-off bath and shower gels and facial scrubbers typically being < 10%. However, it is unclear if the data reported represent products that are currently on the market or relate to historical usage, whereby given a combination of both voluntary and regulatory actions, polyethylene should not be currently used in the majority of products listed. The potential to monitor annual changes in chemical ingredient use in Euromonitor Passport, however, is therefore in contrast to the approach adopted by CPDat, where there appears to be less transparency related to when the information used to populate the underlying product MSDS was produced.

Changes in the use of chemical ingredients in HPCPs are further highlighted in the CIR summaries, which implies a need to consider how temporal changes in chemical ingredients reported in CPDat could potentially be better captured. The issue related to the inability to capture temporal trends in chemical ingredient use represents a potentially significant weakness for CPDat, which may facilitate apprehension regarding underlying uncertainties associated with the relevance of information that might be obtained.

A strength of CPDat, however, is the ability to readily extrapolate information on an individual product level. This level of information could potentially lend itself well to higher-tier evaluations aimed at identifying specific products and product categories where obtaining a refined understanding of consumer use and habits data would greatly strengthen the exposure estimate. This level of information could be further used in helping to identify effective mitigation strategies that target reductions associated with vulnerable use scenarios for priority chemicals. While the ability to scrutinize individual products is recognized as a strength of CPDat, the limited granularity to readily evaluate the use and exposure of chemical ingredients as they relate to individual products represents a potential weakness of the Euromonitor Passport database. Since the approach used in the Euromonitor Passport database relies on populating the database based on products and chemical ingredients that dominate the market, uncertainties will likely accompany estimates of less commonly used chemical ingredients and/or the use of chemicals in less commonly used products, which are identified as being poorly represented in the method used to extrapolate use.

CONCLUSIONS

In summary, the relatively good agreement between the various sources of information evaluated here implies the potential for promising advances toward characterizing and quantifying the exposure of chemical ingredients used in HPCPs. By adopting a complementary approach that optimizes the strengths of the individual methods, improvements to the overall exposure assessment might be realized. For instance, a tiered approach is proposed, whereby the use of chemical ingredients in HPCPs can be estimated using a combination of conservative assumptions, such as the relative weight fraction inclusion level of an ingredient in a product category, coupled with marketing analytic data that report total tonnage volumes of products sold within a geographic region. Screening level tonnage data can thus be used as an emissions input parameter in an exposure model, which, when combined with the physicochemical properties of chemicals, can support an exposure-based screening and prioritization activity by various stakeholders, including industry and government[28-31]. Further refinement of high priority chemical ingredients is possible, whereby individual products for which chemicals are used can be evaluated through the application of CPDat, which, when combined with a refined understanding of consumer use and habit information, would further help reduce the uncertainty that might accompany the tonnage estimate derived based on marketing analytic data.

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Authors' Contributions

The conception, data acquisition and analysis entirely initiated, written, read and approved: Gouin T.

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The author declared that there are no conflicts of interest.

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Not applicable.

Consent for Publication

Not applicable.

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REFERENCES

1. Cowan-Ellsberry CE, Robison SH. Refining aggregate exposure: example using parabens. *Regul Toxicol Pharmacol* 2009;55:321-9. DOI PubMed
2. Gouin T, van Egmond R, Sparham C, Hastie C, Chowdhury N. Simulated use and wash-off release of decamethylcyclopentasiloxane used in anti-perspirants. *Chemosphere* 2013;93:726-34. DOI PubMed
3. Wannaz C, Franco A, Kilgallon J, Hodges J, Jolliet O. A global framework to model spatial ecosystems exposure to home and personal care chemicals in Asia. *Sci Total Environ* 2018;622-623:410-20. DOI PubMed
4. Safford B, Api AM, Barratt C, et al. Use of an aggregate exposure model to estimate consumer exposure to fragrance ingredients in personal care and cosmetic products. *Regul Toxicol Pharmacol* 2015;72:673-82. DOI PubMed
5. Hodges JE, Holmes CM, Vamshi R, Mao D, Price OR. Estimating chemical emissions from home and personal care products in China. *Environ Pollut* 2012;165:199-207. DOI PubMed
6. Gouin T, Avalos J, Meyberg M, Brunning I, Rettinger K, et al. Use of micro-plastic beads in cosmetic products in europe and their estimated emissions to the north sea environment. *SOFW* 2015;141:40-6. DOI

7. Gouin T, Roche N, Lohmann R, Hodges G. A thermodynamic approach for assessing the environmental exposure of chemicals absorbed to microplastic. *Environ Sci Technol* 2011;45:1466-72. DOI PubMed
8. Zhu Y, Price OR, Kilgallon J, et al. Drivers of contaminant levels in surface water of China during 2000-2030: relative importance for illustrative home and personal care product chemicals. *Environ Int* 2018;115:161-9. DOI
9. Goldsmith MR, Grulke CM, Brooks RD, et al. Development of a consumer product ingredient database for chemical exposure screening and prioritization. *Food Chem Toxicol* 2014;65:269-79. DOI PubMed
10. Phillips KA, Wambaugh JF, Grulke CM, Dionisio KL, Isaacs KK. High-throughput screening of chemicals as functional substitutes using structure-based classification models. *Green Chem* 2017;19:1063-74. DOI PubMed PMC
11. Comiskey D, Api AM, Barratt C, et al. Novel database for exposure to fragrance ingredients in cosmetics and personal care products. *Regul Toxicol Pharmacol* 2015;72:660-72. DOI PubMed
12. The Soaps and Detergent Association. Exposure and risk screening methods for consumer product ingredients. 2005. Available from: https://www.cleaninginstitute.org/sites/default/files/research-pdfs/Exposure_and_Risk_Screening_Methods.pdf [Last accessed on 13 Jul 2022].
13. Hall B, Steiling W, Safford B, et al. European consumer exposure to cosmetic products, a framework for conducting population exposure assessments Part 2. *Food Chem Toxicol* 2011;49:408-22. DOI PubMed
14. Hall B, Tozer S, Safford B, et al. European consumer exposure to cosmetic products, a framework for conducting population exposure assessments. *Food Chem Toxicol* 2007;45:2097-108. DOI PubMed
15. Loretz L, Api AM, Barraj L, et al. Exposure data for personal care products: hairspray, spray perfume, liquid foundation, shampoo, body wash, and solid antiperspirant. *Food Chem Toxicol* 2006;44:2008-18. DOI PubMed
16. Loretz LJ, Api AM, Babcock L, et al. Exposure data for cosmetic products: facial cleanser, hair conditioner, and eye shadow. *Food Chem Toxicol* 2008;46:1516-24. DOI PubMed
17. Whelan MJ, Hodges JE, Williams RJ, Keller VD, Price OR, Li M. Estimating surface water concentrations of "down-the-drain" chemicals in China using a global model. *Environ Pollut* 2012;165:233-40. DOI PubMed
18. Gouin T, van Egmond R, Price OR, Hodges JE. Prioritising chemicals used in personal care products in China for environmental risk assessment: application of the RAIDAR model. *Environ Pollut* 2012;165:208-14. DOI PubMed
19. European Chemicals Bureau. Technical Guidance Document on Risk Assessment. European Commission; 2003. Available from: https://echa.europa.eu/documents/10162/987906/tgdpart2_2ed_en.pdf/138b7b71-a069-428e-9036-62f4300b752f [Last accessed on 13 Jul 2022].
20. National Academies of Sciences Engineering Medicine. Exposure science in the 21st century: a vision and a strategy. Available from: https://nap.nationalacademies.org/catalog/13507/exposure-science-in-the-21st-century-a-vision-and-a [Last accessed on 13 Jul 2022].
21. Hubal EA. Biologically relevant exposure science for 21st century toxicity testing. *Toxicol Sci* 2009;111:226-32. DOI PubMed
22. Dionisio KL, Frame AM, Goldsmith MR, et al. Exploring consumer exposure pathways and patterns of use for chemicals in the environment. *Toxicol Rep* 2015;2:228-37. DOI PubMed PMC
23. Phillips KA, Yau A, Favela KA, et al. Suspect screening analysis of chemicals in consumer products. *Environ Sci Technol* 2018;52:3125-35. DOI PubMed PMC
24. Isaacs KK, Phillips KA, Biryol D, Dionisio KL, Price PS. Consumer product chemical weight fractions from ingredient lists. *J Expo Sci Environ Epidemiol* 2018;28:216-22. DOI PubMed PMC
25. Dionisio KL, Phillips K, Price PS, et al. The chemical and products database, a resource for exposure-relevant data on chemicals in consumer products. *Sci Data* 2018;5:180125. DOI PubMed PMC
26. Isaacs KK, Dionisio K, Phillips K, Bevington C, Egeghy P, Price PS. Establishing a system of consumer product use categories to support rapid modeling of human exposure. *J Expo Sci Environ Epidemiol* 2020;30:171-83. DOI PubMed PMC
27. Williams AJ, Grulke CM, Edwards J, et al. The CompTox chemistry dashboard: a community data resource for environmental chemistry. *J Cheminform* 2017;9:61. DOI PubMed PMC
28. Arnot JA, Mackay D, Webster E, Southwood JM. Screening level risk assessment model for chemical fate and effects in the environment. *Environ Sci Technol* 2006;40:2316-23. DOI PubMed
29. Csiszar SA, Ernstoff AS, Fantke P, Meyer DE, Jolliet O. High-throughput exposure modeling to support prioritization of chemicals in personal care products. *Chemosphere* 2016;163:490-8. DOI PubMed PMC
30. Dellarco M, Zaleski R, Gaborek BJ, et al. Using exposure bands for rapid decision making in the RISK21 tiered exposure assessment. *Crit Rev Tox* 2017;47:317-41. DOI PubMed PMC
31. Wambaugh JF, Setzer RW, Reif DM, et al. High-throughput models for exposure-based chemical prioritization in the ExpoCast project. *Environ Sci Technol* 2013;47:8479-88. DOI PubMed