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Problematic chemicals in recycled plastic intended for cosmetics packaging

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Preface

The present report is a follow up on the results from Environmental Project no. 2174 (Danish Technological Institute and DHI A/S, 2021). Here, results of migration analyses of various qualities of post-consumer recycled (PCR) plastic were presented together with an initial safety assessment for a limited number of substances.

In order to conduct a more extensive evaluation of **all** of the migration results, an excel-based screening tool has been developed. Here, the migration results can be matched up against various hazard lists eg. SVHC, CMR, ED, allergy etc.

The project has been carried out with an overall aim to create a so-called 'hotspot'-list, i.e., a limited list of problematic substances, which should be documented are not migrating from PCR. We suggest that this documentation is used in the supply chain communication regarding the PCR quality. The methodology for developing such a list was created through discussions between the Danish Environmental Protection Agency and DHI A/S between October 2021 and September 2022.

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Summary

The present report is presenting the additional work done since the publication of the initial safety assessment (Danish Technological Institute and DHI A/S, 2021)

This additional work comprises the following:

1. Search for other existing guidance documents and the like in recent literature (see appendix 2)
2. Evaluation of other existing guidance documents (see chapter 2).
3. Interpretation and comparison of migration analyses of virgin PE polymers vs. PCR (analyses of virgin PE polymers carried out outside the present project; see chapter 4)
4. Development of an excel-based screening tool for matching migration results with lists of problematic substances e.g. SVHC, CMR, ED, allergy etc. (see chapter 3 and appendix 3)
5. Use of the excel tool to make a comprehensive evaluation of the detected chemicals in the initial safety assessment (Danish Technological Institute and DHI A/S, 2021). The focus of the evaluation is the development of so-called 'hotspot' lists, which we suggest should be used by industry in their supply chain communication to document the PCR quality especially regarding the absence of a limited number of substances with problematic hazard properties.

We have developed two hotspot lists for PCR to be used for packaging of cosmetics: One for leave-on products and one for rinse-off products. The hotspot list for leave-on products comprises 28 substances or groups of substances, whereas the hotspot list for rinse-off products comprises 11 substances.

The lists have been developed after considerations concerning:

- Worst case exposure
- Maximum found migration from PCR performed in an earlier project
- Appearance of the substances on various hazard lists
- Toxicological assessments resulting in TDI, DNEL, TTC etc.
- Absorption through skin
- Skin sensitisers
- Comparison of migration results from PCR and virgin PE plastic
- Other guidance documents and ongoing work on PCR for cosmetic packaging

Initially the hotspot lists were planned to be found using an excel screening tool developed as part of the project. Here substances on various hazard lists can be matched up against a given dataset. In the end, most of the hotspot substances were identified as the result of a risk-based analysis, where the measured concentration of the substances was compared with a calculated maximum acceptable concentration depending on a leave-on or rinse-off type of cosmetic product.

The excel screening tool may be used as an aid to deal with the multitude of substances often being the result of migration analyses of PCR.

The hotspot lists are a tool to demonstrate the non-presence of a limited number of problematic substances in PCR intended for cosmetic product packaging. We suggest that this documentation of the PCR quality is communicated in the supply chain for the cosmetic product. However, it does not free manufacturers of cosmetic products of the duties to 1) perform

safety assessments of the packaging containing PCR 2) to adhere to other regulatory instruments such as the absence of e.g. CMR-substances in cosmetics and conforming with PAH/PAA restrictions. General guidance for providing information on PCR in the supply chain for cosmetic product packaging can be found in the guidance documents mentioned in chapter 2.

1. Introduction

1.1 Objective

Assessing the safety of post-consumer recycled plastic (PCR) in contact with cosmetic products is difficult, because of the immense numbers of substances which may migrate from the plastic packaging into the cosmetic product. It is advantageous to try and limit the analytical workload and the subsequent safety assessment to manageable levels. This may be done by pointing out a limited number of 'hotspot' substances in PCR in relation to packaging of cosmetic products. By 'hotspot' substances we mean substances, which are problematic regarding their hazard profile to such an extent that their absence in the PCR raw material is an important quality parameter for the supply chain communication on the packaging of cosmetic products.

Acceptable concentrations in PCR packaging may differ from product type to product type of cosmetics, most notably between rinse-off and leave-on products. Developing criteria for making a list of such hotspot substances is therefore the prime objective of this project.

In this report, we provide the technical basis for developing criteria for two lists of hotspot substances, one for leave-on products and one for rinse-off products. The lists of hotspot substances are not exhaustive and does not alleviate the company of performing proper safety assessments of all other migrating substances and conform to other regulations such as 1) avoid CMR in cosmetics products 2) restrictions on PAA and PAH. Conversely, the lists of hotspot substances are intended as an aid to preclude and document absence of a limited number of problematic substances that we know can occur in PCR. We suggest that this can be used as an element in the quality documentation for the supply chain communication.

1.2 Background

Previously, the Danish Environmental Protection Agency (Miljøstyrelsen, MST) has funded and published the results of a study on migration of substances from samples of PCR and an initial safety assessment when used as packaging in contact with cosmetic products (Danish Technological Institute and DHI A/S, 2021), which we refer to as Environmental Project no. 2174. The aim of that project was to generate knowledge and data on PCR plastics, to contribute to creation of guidelines for the cosmetics industry on how PCR plastic can be safety assessed and used safely for packaging of cosmetic products for personal care (e.g., shampoo, body lotion or liquid hand soap).

In addition to analytical laboratory screenings, specific laboratory analyses were performed for selected substances/groups of substances, which were considered relevant in relation to the safety assessment of PCR plastic material. The selected substances do not constitute an exhaustive list of substances relevant to analyse in connection with a safety assessment of PCR plastic materials. Rather, the substances were prioritized based on the experience and knowledge of the project group on PCR plastic, problematic substances, and available analysis methods.

The following substances were selected for substance-specific laboratory analyses:

- Polycyclic aromatic hydrocarbons (PAH), as they were previously found in products of recycled plastic and are considered carcinogenic upon skin contact.

- Primary aromatic amines (PAA), as they were previously found in food contact materials of recycled plastic. These are considered carcinogenic and are subject to restrictions in, for example, legislation on food contact materials.
- Possible degradation products of antioxidants and stabilizers (often referred to as 'phenol (PE)', even if the group also includes substances without a phenol-structure), which according to experience from, among others, measurements in drinking water pipes, can migrate out of PE-plastic. These include substances, which affect liver and kidneys and are suspected of having a damaging effect on genetic material.
- Perfluoroalkyl and polyfluoroalkyl substances (PFAS), which may be absorbed from other PFAS-treated products and may have toxic effects on reproductive system, immune system, persistent and neurotoxic effects.

In total, around 317 substances were identified, most of them down to CAS number. In the following this dataset will be referred to as the migration dataset.

Out of this dataset, an initial safety assessment was performed for a limited number of substances.

The present report is presenting the additional work done since the publication of Environmental Project no. 2174 in order to make a more comprehensive evaluation taking into account all of the migrants detected in the previous project.

This additional work comprises the following:

1. Search for other existing guidance documents and the like in recent literature (see appendix 1)
2. Evaluation of other existing guidance documents (see chapter 2).
3. Interpretation and comparison of migration analysis of virgin PE polymers vs. PCR (analysis of virgin PE polymers carried out outside the present project) (see chapter 4)
4. Development of an excel-based screening tool for matching migration results with lists of problematic substances e.g. SVHC, CMR, ED, allergy etc. (see chapter 3 and appendix 3)
5. Use of the excel tool to make a comprehensive evaluation of the detected chemicals in in Environmental Project no. 2174. The focus for the evaluation is the development of so-called hotspot lists, which can be used by industry in their supply chain communication to document the PCR quality especially regarding the absence of a limited number of problematic substances. The evaluation includes a risk-based analysis and some further additional considerations regarding some selected chemical groups (sensitisers, phthalates, CMR, PAH, PAA).

At present, it is practice in the cosmetic product industry to accept plastic intended for food as safe to use for cosmetic products (see chapter 2.1. The Cosmetics Europe advisory document, 2019). This practice is difficult to apply to PCR, because:

- PE and PP-PCR is usually not of a quality which fulfil the requirements for food contact materials and has not been approved as such.
- PE and PP-PCR can potentially contain hundreds of substances which may migrate into the cosmetic products.
- It is difficult to distinguish non-intentionally added substances (NIAS) in PCR from those which are normally occurring in virgin plastic.

List of terms and abbreviations

ADI	Acceptable Daily Intake
Bw	Body Weight
CMR	Carcinogenic, Mutagenic and Reprotoxic. CMR-substances are carcinogenic, mutagenic and reprotoxic substances.
DMEL	Derived Minimal Effect Level
DNEL	Derived no-effect level
FCM	Food Contact Material
MoS	Margin of Safety
NIAS	Non-intentionally added substances (=contaminants)
PE	Polyethylene
PP	Polypropylene
REACH	Registration, Evaluation, Authorization and Restriction of Chemicals, Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
SCCS	Scientific Committee on Consumer Safety - EU's scientific committee for consumer health and safety
SVHC	Substance of very high concern
TDI	Tolerable Daily Intake refers to the daily amount of a chemical that has been assessed safe for daily intake for human being on a long-term basis (used in case of contamination)
TTC	Threshold of Toxicological Concern refers to the lowest exposure that may cause a toxicological effect. TTC may be used as the tolerable daily intake of substances with missing toxicological data.

2. Other existing guidance documents and the like found in recent literature

Two existing guidance documents about safety assessment of PCR for use as packaging material for cosmetic products were identified: The Cosmetics Europe advisory document from 2019, and a Cosmetic Packaging Guidance prepared by Fraunhofer et al. from February 2021. A literature search for other, similar guidance documents was carried out, and the search strategy and results are presented in Appendix 1.

It should be noted that the content of these guidance documents does not necessarily agree with the opinion of competent authorities.

In addition, we have learned that there is an industry working group, called Cospatox, whose aim is to accomplish the so far missing specific safety standards for high-quality PCR for cosmetics and other household packaging as well as the implementation of on-site measurement methods for recyclers.

In the following, these two documents and the Cospatox work are briefly summarized. A discussion of their usefulness is given in the last section of this chapter.

2.1 The Cosmetics Europe advisory document, 2019

The advisory document (Cosmetics Europe, 2019) concerns information exchange on cosmetic packaging materials along the value chain in the context of the EU Cosmetics Regulation (no. 1223/2009). It points out the substances of concern to cosmetic safety assessors as follows:

Substances of concern	Reporting thresholds
Substances specifically banned or restricted in Annex II or III of the Cosmetics Regulation, including CMR-substances	10 ppm in the material or 100 ppb migrating level
Substances classified as skin sensitisers according to CLP Regulation, Annex VI table 3.1 Annex VI table 3.1	When present at above 0.1 % (for skin sensitisers Cat 1B or 1) or 0.01 % (for skin sensitisers Cat 1A) or, alternatively, when migrating in a relevant simulant in levels above 100 ppb or 1000 ppb for sensitisers categorised as Cat 1A or 1/1B, respectively

The guidance document states that communicating the occurrence of substances of specific concern (namely those on Annex II or III) to cosmetic safety assessors should be addressed by:

- Statement on ‘no intentional addition or known presence’ OR
- Information on substances (name, CAS no., max. concentration)

Furthermore, reportable substances under REACH and Packaging Waste Directive no. 94/62 (heavy metals) should be mentioned by name, CAS no. and max. concentration.

Supplier statements of compliance with the food contact materials (FCM) legislation should be given, including:

- Condition/type of food under which the statement is valid
- Type of information available on migration (e.g. test with food/simulant, modelling, worst case assumptions)
- Substances with migration limits (name, CAS no., max. concentration in the packaging component or material)

If the material is non-compliant with FCM legislation, reason and, where applicable, name, CAS-no, and max. concentration of the non-compliant substances in the material should be given. This would be the case for most PCR made of PP or PE.

The advisory document is accompanied by an excel tool listing 'disclosable substances' (i.e. substances to be disclosed by the material/packaging manufacturer to the next person in the chain of supply). The excel-file for the guidance list was built as shown in the figure below (from the advisory document).

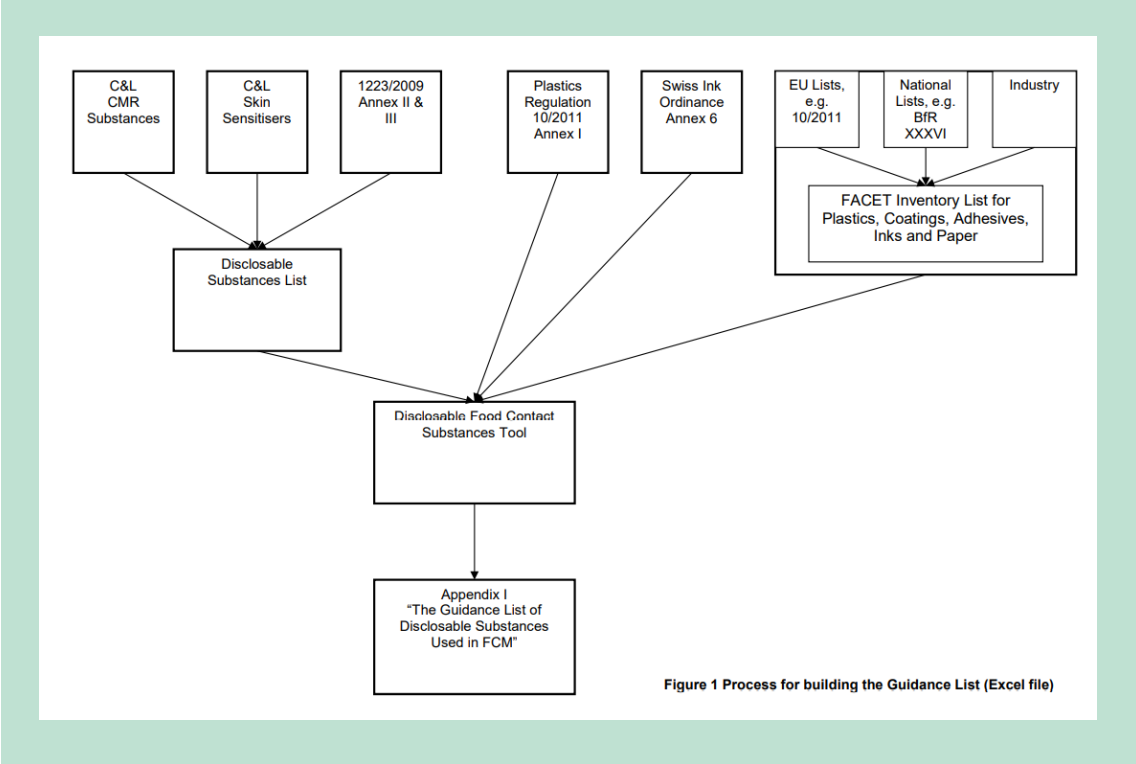

FIGURE 1. Process for building the Guidance List (Excel file from Cosmetics Europe).

In Figure 1 it can be seen that the list of disclosable substances is composed of substances classified as CMR-substances, skin sensitisers and substances restricted in cosmetics according to the Cosmetics Regulation, Annex II and III. In addition, the substances listed in the Plastic Food Contact Regulation (10/2011), Annex I, the Swiss Ink ordinance annex 6[1], and the FACET Inventory list for Plastics, Coatings, Adhesives, Inks and Paper (Food Packaging Forum, 2014)) are included.

[1] The Swiss Ink ordinance specifies the materials and articles intended to come into contact with foodstuffs and lays down the requirements relating thereto.

The FACET inventory list is based on the following data:

- Regulation (EU) 10/2011, which sets out safety requirements for plastic materials and articles intended to come into contact with food
- BfR XXXVI, Recommendation for paper and board for food contact
- Industry developed requirements

2.2 Cosmetic Packaging Guidance prepared by Fraunhofer et al. from February 2021

The intention of the document is to summarize the knowledge on post-consumer contaminants in HDPE and PP recyclates and consumer safety evaluation. This should give practical guidance and reliable criteria for the safe use of post-consumer HDPE and PP recyclates in cosmetic packaging. In particular, the maximum concentrations of post-consumer contaminants in cosmetic packaging should be given, which can be used in routine control to assure the high-quality standards of cosmetic packaging materials (Pereda, Gerber, Sander, & Welle, 2021).

According to the guidance, manufacturers of cosmetic products consider the packaging to be safe if food compliance can be confirmed according to Regulation (EU) No 10/2011 and Regulation (EC) No 1935/2004 on food contact materials. However, since this is usually not possible for post-consumer recyclate materials, the company must prove the safety of these materials for cosmetics by evaluating all toxicological endpoints of any migrating substance. A batch-related control of the post-consumer materials by means of analysis and the evaluation of the substances found, either directly in the material or after migration tests in the respective product, is mandatory. Based on the concentrations found in the materials, a toxicological evaluation can be applied, e.g. by evaluating the specific toxicity of any impurity or by applying the threshold limits of the TTC approach[2]. By means of examples, detection limits needed for rinse-off and leave-on products of 12 mg/kg and 3 mg/kg, respectively, are calculated. Non-identified substances should be below these threshold limits. It's important to note, that a general threshold limit cannot be applied, because the detection or threshold limits depend on the exposure scenario. In addition, the necessary detection limits depend on the recyclate amount in the final packaging, the volume of the packaging and the packaging weight. Therefore, the detection limits necessary for compliance evaluation depends on exposure of the consumers to the specific cosmetic product.

2.3 Cospatox

CosPaTox Consortium counts 38 major European brand owners of the cosmetic industry, hygiene and detergents & cleaning agent sector, committed recycling companies, plastic manufacturers and plastic convertors (Cospatox, 2021). They have partnered up with:

- Fraunhofer Institute for Process Engineering and Packaging IVV
- University of Applied Sciences Vienna
- Fabes Forschungs-GmbH for Analytic and Evaluation of Mass Transfer Processes

CosPaTox states that the use of recyclates in the context of a growing circular economy is, with a few exceptions, limited to the approved food-grade recyclates for which there are legal regulations.

CosPaTox seeks to define toxicological safety guidelines for PCRs used in cosmetics packaging, with a first focus on polyolefins (rPE-HD, rPE-LD and rPP; if time and budget allows also PET). Three different types of packaging are in the focus of CosPaTox:

[2] See chapter 4.3 for more information about TTC

- Leave on cosmetics,
- rinse-off cosmetics and
- Wash- and cleaning detergents.

The aim is to establish a test strategy and a dossier to facilitate the implementation of an EU voluntary industry standard.

2.4 Discussion

The two guidance documents are much in line with the analysis work and recommendations found in Environmental Project no. 2174 (Danish Technological Institute and DHI A/S, 2021).

The guidance list provided by Cosmetics Europe includes some of the same lists as the excel-tool for screening of substances developed in this project. However, our excel tool (described in the next chapter) also includes the REACH restricted substances, the SVHC, the SIN list, endocrine disruptors, and STOT RE classified substances. The Cosmetics Europe guidance list is useful as a reference when exchanging information on cosmetic packaging materials. It is leaning much against the established system of declaration of compliance with FCM legislation, although it also states that, "*It does not provide safety assessment methodologies for integrating such information into the cosmetic product safety assessment. This remains fully in the role of the cosmetic product safety assessor*." The guidance document does not specifically consider packaging materials made of PCR.

The Fraunhofer et al. guidance calculates needed detection limits for rinse-off and leave-on products of 12 mg/kg and 3 mg/kg, respectively, based on TTC and exposure of adults, where Environmental Project no. 2174 finds 49 µg/kg and 0.8 µg/kg based on TTC and worst-case exposure scenarios for babies. Possibly, the reason for this difference (a factor 1000) is that Fraunhofer et al. uses a scenario with exposure of an adult and larger packaging size (more volume in relation to packaging material) whereas the scenario in Environmental Project no. 2174 is exposure of a baby with lotion from small packaging (less volume in relation to packaging material), and in addition we apply a 10% allocation factor to cosmetic packaging, since the consumer may be exposed to the same substances from other sources, such as drinking water, food and medical supplies.

Finally, we note that Cospatox also seems to rely on approved food grade recyclates. This is not necessarily a good idea, since some substances may be more critical in contact with skin than when ingested.

3. Excel-tool for screening of substances

During the Environmental Project no. 2174, a long list of substances identified in recycled plastic materials to be used as packaging materials for cosmetic products were found by chemical analysis (= “the migration dataset”). A human risk assessment of a few of these substances was carried out. However, no further assessment was done for the rest of the substances, and a hazard screening of these remaining non-assessed substances may give an overview of, whether some of these substances are of concern. Therefore, DHI A/S was requested to develop an excel-based tool, where the substances in the migration dataset could be matched up against various lists of problematic substances. The details of these lists can be found in Table 1, and a comprehensive description of the excel tool can be found in appendix 3.

In Figure 2 is shown an example of an analysis made with the new excel tool on a reduced set of substances in the migration dataset.

	Substances used in plastic (packaging)			Problematic substances												Classification	
Component	PLASI	FCM	CPPdb	SVHC	XVII	ED1	ED2	CMR	STOT RE	Allergy (class.)	Fragrances	COS2	COS3	SIN	RSL	HAR	ADV
2,4-Dimethylheptane or isomer																	
Diethylhexyl phthalate (DEHP)																Repr. 1B;	
1,6-Hexanediol diacrylate (HDDA)																Skin Irrit. 2; Eye Irrit. 2; Skin Sens. 1;	
1-Butoxy-2-propanol																Skin Irrit. 2; Eye Irrit. 2;	
1-Decanol																	Skin Sens. 1
1-Tetracosene (C24:1)																	Skin Sens. 1
2,2,4,4,6,8,8-Heptamethylnonane																	Skin Irrit. 2
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB)																	Repr. 2; Aquatic Acute 1; Aquatic Chronic 1
2,4,5-trimethylaniline																	Carc. 2; Muta. 2; Acute Tox. 4; Skin Sens. 1
2,4-diaminoanisol																Carc. 1B; Muta. 2; Acute Tox. 4 *; Aquatic Chronic 2;	
2,4-Diaminotoluene																Carc. 1B; Muta. 2; Repr. 2; Acute Tox. 3 *; Acute Tox. 4 *; STOT RE	
2,4-Diethyl-9H-thioxanthen-9-one																	Acute Tox. 4
2,4-di-tert-butylphenol																	Aquatic Acute 1; Aquatic Chronic 1
Butylated Hydroxytoluene																	Muta. 2; Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2; Aquatic Acute 1;
α-Hexylcinnamaldehyde																	Skin Sens. 1; Skin Irrit. 2; Aquatic Acute 1; Aquatic Chronic 1
n-Hexyl salicylate																	Aquatic Acute 1; Aquatic Chronic 1
α-Pinene																	Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1

FIGURE 2. Example of an analysis made with the excel tool on a limited number of substances from the migration dataset.

Each substance is matched up against four types of information (see Table 1 for a more detailed description of the individual lists):

a. Existing lists of chemical substances known to be used in **plastics (PLASI, FCM, CPPdb)**. A grey box indicates that the specific substance can be found on this list. E.g. DEHP is found on FCM.

b. Existing list of **chemical substances of concern** (SVHC, XVII, ED1, ED2, COS2, CO3, SIN, RSL). A red box indicates that the specific substance can be found on this list. E.g. DEHP is also found on SVHC, XVII, ED1, COS2 and SIN).
c. For each substance the harmonized **classification** (HAR) and advisory list for self-classification of hazardous substances (ADV) is included. The columns CMR, STOT RE and Allergy are based on the classification text and if the individual substance contains this endpoint, and if it is found on the harmonized or the advisory list, respectively, a dark or a light red box is indicated in the three columns. As an example, DEHP has the harmonized classification Repr. 1B and therefore a *dark* red box is indicated under the CMR column. Furthermore, 1-Decanol has the advisory classification Skin Sens. 1 and therefore a *light* red box is indicated under the Allergy column.
d. F**ragrances** which are included in either of the following groups (i) declarable (ii) under considerations regarding declaration **or** (iii) residual group of fragrances. The presence of a given substance in any of these three groups are indicated respectively with a dark red, light red and grey box. As an example, α-Hexylcinnamaldehyde is on the existing list of declarable fragrances (dark red box), α-Pinene is in the group of considerations for declaration (light red box) and n-Hexyl salicylate is in the residual group (grey box).

The full analysis of all the substances in the migration dataset can be found here: https://mst.dk/media/256345/excel-analysis_recycled-plast.xlsm
It shows that there are a lot of substances in the migration dataset with problematic properties. Initially the further hotspot analysis was planned to be done on substances from each hazard group. However, as it turned out (see chapter 5), most of the hazard groups could be analysed collectedly under the risk-based analysis. Only results shown in the two columns Allergy and Fragrances were actively used in the hotspot analysis.

Regardless of this limited use of the excel tool in this project, it is still available for ad hoc evaluations of large groups of substances of unknown hazard profile. Presently, the migration dataset from the Environmental Project no. 2174 is inserted in the excel tool, but other datasets may be inserted in the excel tool.

TABLE 1. Overview of Public lists included in the tool (as of April, 2021)

Theme	Description of list
Substances used in plastic A grey box indicates that the substance appears on the list.	PLASI (Plastics additives initiative, https://echa.europa.eu/da/plastic-additives-initiative) PLASI lists over 400 additives in plastics used in high volumes in the EU. It should be noted, that this relates to all plastic materials, including, but not only for those meant for food contact. In this context, "additive" means a substance which is intentionally added to plastics to achieve a physical or chemical effect during processing of the plastic or in the final material or article; it is intended to be present in the final material or article. Dyes, slip promoters, and polymeric impact modifiers were not covered in the search. FCM: Union list of authorized monomers, other starting substances, macromolecules obtained from microbial fermentation, additives and polymer production aids Commission Regulation (EU) No 10/2011 on plastic materials and articles intended to come into contact with food (Annex I) Annex1 to (EU) No 10/2011[3] Union list of authorized monomers, other starting substances, macromolecules obtained from microbial fermentation, additives and polymer production aids. This is a so-called positive list, meaning that only the

[3] EUR-Lex - 02011R0010-20200923 - EN - EUR-Lex (europa.eu)

	substances mentioned in this list may be used in plastic intended for food contact. The list also specifies specific migration limits and other conditions for the application of the substances. The list does not comprise colorants; solvents; certain salts of authorized acids, phenols or alcohols; polymers with a weight of 1000 kDa or more; and aids to polymerization. CPPdb (Chemicals associated with Plastic Packaging, Food Packaging forum, from https://zenodo.org/record/1287773#.YEnMwThYZZV The CPPdb covers both food and non-food packaging. It currently contains 3377 chemicals that are possibly associated with plastic packaging.
Classification	Classification (no H-phrases specified) HAR: List of harmonised classification (EU) in force from 9 September 2021, which was taken from: https://echa.europa.eu/documents/10162/17218/annex_vi_clp_table_atp14_en.xlsx/c767afd2-4d53-b8d5-de2b-0820680cac95 ADV: The advisory list for self-classification of hazardous substances, found on https://mst.dk/kemi/kemikalier/stoflister-og-databaser/vejledende-liste-til-selvklassificering-af-farlige-stoffer/. The list is provided by the Danish Environmental Protection Agency to aid businesses in self-classification. The list includes more than 54,000 substances.
Problematic substances A red box indicates that the substance appears on the list. For the following lists, the match is further differentiated: 1) CMR, STOT and Allergy 2) Fragrances (see further details in the table)	SVHC (Substances of Very High Concern). The list is taken from the ECHA website (https://echa.europa.eu/da/candidate-list-table) REACH Restriction list, Annex XVII. This list is taken from the ECHA web-site (http://echa.europa.eu/addressing-chemicals-of-concern/restrictions/substances-restricted-under-reach) Endocrine Disruptors ED1: Substances identified as endocrine disruptors at EU level ED2: Substances under evaluation for endocrine disruption under an EU legislation. The lists are taken from https://edlists.org/the-ed-lists Substances with a harmonized classification with: CMR STOT RE ALLERGY (Skin Sens) For all endpoints, all subcategories are be included (ex. 1,1a,1b). A dark red box indicates that a substance has a harmonized classification with this end point. Substances with a classification from the advisory list of classification with: CMR STOT RE ALLERGY (Skin Sens) For all endpoints, all subcategories are be included (ex. 1,1a,1b). A light red box indicates that a substance has an advisory classification with this end point. Commission Regulation (EC) No 1223/2009 on cosmetic products COS2: List of substances prohibited in cosmetics products (Annex II) COS3: List of substances which cosmetic products must not contain except subject to the restrictions laid down (Annex III) SIN list, ChemSec The SIN list is a comprehensive list of substances that has been identified by ChemSec as fulfilling the criteria for Substances of Very High Concern (SVHC), as described in the EU chemicals regulation REACH article 57: CMR, PBT/vPvB and “substances of similar concern” (ED, specific organ toxicity, allergenes, PMT, vPvM). The list is retrieved from https://sinlist.chemsec.org/ RSL Restricted Substance List, ref. Cradle to Cradle (se link) The Cradle to Cradle Products Innovation Institute is a non-profit organization that maintains a standard for products and materials to become ‘Cradle to Cradle certified’. This is a certification for sustainable products and certifies them as safe, responsible, and fit for a circular economy. The Restricted Substances List (RSL)

	is a checklist for materials that are not allowed to be used in certified products. The list is comprised of restrictions on chemicals from multiple existing chemical regulations such as the one mentioned above. The most conservative thresholds for each substance in any of the combined regulations is chosen. The list is retrieved from https://www.c2ccertified.org/resources/detail/cradle-to-cradle-certified-banned-list-of-chemicals
Fragrances	Three groups of fragrances are included in the excel tool: A group of 26 fragrance allergens subject to individual labelling according to the Cosmetics Regulation (annex III of Regulation no. 1223/2009). These fragrances should be declared on the ingredient list if intentionally used in cosmetic products above a specific concentration limit. In the following, this group is referred to as declarable fragrances, and a dark red box indicates that a given substance is included in this group. Fragrances listed in Table 13.1 of SCCS (2012) excluding group 1 above. A future declaration requirement for some of these substances are currently discussed under the auspices of amendments to the Cosmetics Regulation. In the following, this group is referred to as fragrances under consideration regarding declaration, and a light red box indicates that a given substance is included in this group. Fragrances listed in Tables 13.2-13.4 of SCCS (2012). These substances have less evidence as established contact allergens in humans. In the following, this group is referred to as the residual group, and a grey box indicates that a given substance is included in this group.

For the substances found in the analyses of Environmental Project no. 2174, information on DNEL or DMEL oral, general public, dermal general public, dermal workers, and dermal absorption was added to the tool after retrieval of the data from ECHA. If dermal absorption was not available an estimated value was added (see appendix 3.5).

4. Comparison of migration from virgin and PCR PE samples.

In the Environmental Project no. 2174, a large number of compounds was detected in the migration from PCR PE samples. It was speculated, that if an analysis of virgin PE samples also showed the same complexity, the safety assessment requirement to the use of PCR PE for packaging of cosmetics products should be extended to the virgin PE samples. It was therefore decided to analyse three commercially available virgin PE samples in a similar way to what was already done on the PCR PE samples in the previous project. The virgin PE samples were obtained from large suppliers of PE for packaging materials. The analysis was carried out outside of the present project and the details of the work can be seen in Appendix 2.

The components found in an analysis of three virgin PE samples consist of two categories:

1. Linear aliphatic compounds (C10-C34, with even numbers of carbon atoms). In sample 970130-1 the dominant compounds were saturated alkanes, whereas the dominant compounds were unsaturated alkenes in sample 970130-2 and -3. This probably has to do with variations in processing, time and temperature. It is very likely, that these compounds are the parts of the molecular weight distribution for the PE polymer, which is small enough to migrate into the product simulant.
2. Various well known plastic additives and/or their degradation products ("PE-phenols"). Examples of antioxidant and stabilizer additives found in highest concentration indicating intended addition are:

    - 970130-1: Tris-(2,4-di-t-butylphenyl) phosphite (CAS no 31570-04-4; concentration 150 ppm)
    - 970130-2: 2,6-Di-tert-butyl-4-[(2-octadecyloxycarbonyl)ethyl]phenol (Irganox 1076) (CAS no 2082-79-3; concentration 26 ppm)
    - 970130-3: Tris-(2,4-di-t-butylphenyl) phosphite (CAS no 31570-04-4; concentration 220 ppm)

The remaining compounds identified in the semi-quantitative GC-MS analysis and the specific "PE phenols" analysis all belong to the group of degradation products for antioxidants and stabilizers and were found in concentrations below 20 ppm.

No PAH components were found in the analysis of the virgin PE samples.

Hence, the conclusion from the comparison is that the compounds found in the analysis of virgin PE all have an explanation. The complexity observed in the analysis of the migration from PCR PE samples was not repeated, and the additional substances found in the PCR samples should therefore be further investigated in any safety assessment of the use of these qualities for packaging of cosmetics products.

5. Method of developing a hotspot list

The principle behind a hotspot list is for it to identify problematic substances, which industry as a minimum should document are not migrating from PCR qualities used as packaging material for cosmetic products.

The number of relevant problematic substances could potentially be counted in thousands. Hence, the development of the present hotspot list should be taken as an attempt to identify a limited number of problematic substances observed to be migrating from PCR in the earlier Environmental Project no. 2174.

The documentation for the absence of substances on the hotspot list cannot be used as a documentation for a complete safety assessment of all possible migrants from a PCR packaging to a certain cosmetic product. Rather, it is envisaged as an aid in the supply chain communication for industry and could for instance be included as part of the specific documentation of commercial PCR qualities.

The hotspot list identified in this project contains the most problematic substances found as migrating from the PCR samples evaluated in Environmental Project no. 2174. The identification of these is mainly based on risk-assessment principles, where the *actual maximum measured concentration*[4] of the substance found to be migrating from PCR is compared with a *maximum calculated acceptable concentration* (see chapter 5.2). The hotspot list collects substances, where the maximum *measured* concentration is larger than the maximum *calculated* acceptable concentration. In addition to these substances, two other groups of substances were also included in the hotspot list: 1) a few fragrances and 2) a selected group of phthalates.

The total number of substances found migrating from PCR in Environmental Project no. 2174 was 319 most of which was identified with a unique CAS number. In the following, we will refer to this list of substances as the total migration dataset. From this dataset, the following substances were not included in the further analysis:

a. Substances not identified unambiguously by a unique CAS number
b. Substances without a measured concentration
c. Substances, which corresponds to the low-molecular part of the normal molecular weight distribution of virgin PE (i.e. C10-C34 alkane/alkenes). These substances are found also as migrating from virgin PE (see section 4.5).

A total of 127 substances remained and was included in the further analysis for populating the hotspot list. In the following, this list will be referred to as the *reduced* migration dataset.

We present here two versions of a hotspot list: One for leave-on products and one for rinse-off products. The number of problematic substances for leave-on products will be larger than for the rinse-off products, as systemic exposure is higher in leave-on products.

[4] Several PCR samples were evaluated in the Environmental Project 2174, and in some cases the same substance was found using different analytical measurement. For each substance only one *measured concentration* was selected for the analysis: the *maximum concentration measured* in either of the PCR samples or either of the analytical techniques.

5.1 Exposure scenarios

Two exposure scenarios were chosen as basis for the analysis for the two versions of the hotspot list:

d. The leave on hotspot list was based on the scenario of exposure to baby body lotion
e. The rinse-off hotspot list was based on the scenario of exposure to baby shampoo

In both cases, a ***baby*** exposure scenario was selected in order to make the most conservative selection of candidates for the hotspot list.

The parameters below have been identified in the previous Environmental Project no. 2174.

Basic data for baby bodylotion (SCCS, 2018)

Average body weight), baby, **K**:.....3.4 kg
Exposure route: .....Dermal
Kind of exposure: .....Leave-on
Quantity per skin surface area $\mathbf{G_A}$: .....0.5 mg/cm^2 (adult, Table 2A&3; 7.82g/15670cm^2)
Daily frequency of application **F**: 1
Surface area per application **A**: .....2200 cm^2 (Cato, 2020)
Retention factor **R**: 1
Dermal absorption fraction/Percutaneous permeation **P**: .....Dependent on the substance

Dermal eposure, E_{dermal}

$E_{dermal} = (G_A * A * F * R) / K = (0,5 * 2200 * 1 * 1) / 3,4 = 323,5$ mg baby body lotion /kg bw/day

In addition, we consider the scenario of exposure to shampoo in combination with shower gel for adults but adjusted afterwards to fit babies by adjusting for surface area.

Basic data for shampoo (adults) (SCCS, 2018)

Average body weight, **K**: .....60 kg
Exposure route: .....Dermal
Kind of exposure: .....Rinse-off
Quantity per day, shower gel $\mathbf{G_{SG}}$:.....18.67 g/day
Quantity per day, shampoo $\mathbf{G_{SH}}$: .....10.46 g/day
Retention factor, shower gel $\mathbf{R_{SG}}$: 0.01
Retention factor, shampoo $\mathbf{R_{SH}}$: 0.01
Dermal absorption fraction/Percutaneous permeation **P**: .....Dependent on the substance

Dermal exposure, E_{dermal} (adult)

$E_{dermal} = (G_{SG} + G_{SH})* R_{SG+SH} / K = (18.67+10.46) * 0.01/ 60 = 4.86$ mg shampoo /kg lgv/day

Dermal exposure, E_{dermal} (baby)

$E_{dermal} = ((A_{baby}/A_{adult})*G_{SG} + G_{SH})* R / K = ((2200/17500)*18,67+10,46)*0,01/3,4 = 37,7$ mg shampoo/kg bw/day

The exposure of babies to shampoo and shower gel is not very well quantified. Data from a Korean study (Lee & al., 2017) exist, but for our purpose of creating a hotspot list, we consider the above approximation of E_{dermal} (baby) as sufficient.

5.2 Calculation of the maximum acceptable concentration

The Margin of Safety (MoS) is Point of Departure (PoD) divided by the Systemic Exposure Dose (SED). Often the NOAEL-value is used for the PoD. Therefore normally (SCCS, 2018), the margin of safety (MoS) is calculated as the ratio of the NOAEL-value to the systemic exposure dose (SED), i.e.

$$MoS = \frac{NOAEL}{SED}$$

The systemic exposure dose (SED) depends on the dermal absorption fraction (P), and is calculated as:

$$Systemic\ exposure\ dose;\ SED = \left(\frac{Conc}{100}\right) * P * E_{dermal}$$

Here, we apply the DNEL instead of NOAEL, because the DNEL already contains the appropriate uncertainty factors in relation to data quality, critical study duration etc., and in the screening tool, we have inserted DNEL values (or TDI or ADI) found in the ECHA database.

A MoS of at least 100 is normally accepted when using NOAEL, but when using DNEL (or TDI or ADI) we only need a MoS of 10 to account for the 10% allocation of DNEL to cosmetic products, to allow for exposure to the same chemical substance from other sources, such as drinking water and food.

With a MoS of 10, we can derive the following maximum calculated acceptable concentration, C:

$$\mathrm{C}(\%) < \frac{100 \cdot \mathrm{DNEL}}{10 \cdot \mathrm{P} \cdot \mathrm{E}_{dermal}} = \frac{10 \cdot \mathrm{DNEL}}{\mathrm{P} \cdot \mathrm{E}_{dermal}}$$

If we, for example, make the calculation for DEHP in baby body lotion, we apply the following values:

- DNEL = 0.05 mg/kg bw/day
- P = 0.05
- E_{dermal} = 323,5 mg/kg bw/day (for a baby)
-

$$\mathrm{C}(\%) < \frac{10 \cdot 0.05 \frac{\mathrm{mg}}{\mathrm{kg\ bw\ day}}}{0.05 \cdot 323{,}5 \frac{\mathrm{mg}}{\mathrm{kg\ bw\ day}}} = 0{,}0309\%$$

or 309 mg/kg baby body lotion.

Likewise, the acceptable maximum concentration for migrants in shampoo was found for each migrant by applying E_{dermal} = 37,7 mg shampoo + shower gel/kg bw/day.

The calculated maximum concentrations were compared to the measured maximum concentration of the 127 migrants in the reduced migrant dataset. In principle, larger concentrations of migrants found than acceptable, leads to inclusion on the hotspot list. Subsequently, the hotspot list was modified by applying certain other considerations as described in chapter 5.5.

5.3 Key parameters: DNEL and P and their substitutes

In cases where no literature value of the dermal absorption fraction, P, was found, it was predicted by the FiniteDoseSkinPerm program (CDC/NIOSH, 2022). If this was not possible, the dermal absorption fraction was assumed to be 1.

If $DNEL_{oral}$ or TDI/ADI values are found, these are applied in the calculations.

If a $DNEL_{dermal}$ is found, it can be used instead but without modification with the dermal absorption fraction (P).

If no $DNEL_{oral}$; TDI/ADI or $DNEL_{dermal}$ values were found, the 'Threshold of Toxicological Concern' (TTC) is applied.

The TTC can be differentiated by applying the Cramer classification, i.e. a classification of the substance according to its chemical structure (Kroes & al., 2007). To get help making a Cramer classification the programme Toxtree may be used.

TABLE 2. The Cramer classification scheme for estimating the TTC based on chemical structure (Kroes & al., 2007)

Cramer Class	Description	TTC [µg/person/day]*
I	Substances of simple chemical structure with known metabolic pathways and innocuous end products which suggest a low order of oral toxicity.	1800 (30 µg/kg bw/day)
II	Substances are intermediate. They possess structures that are less innocuous than those in Class I but they do not contain structural features that are suggestive of toxicity like those in class III.	540 (9 µg/kg bw/day)
III	Substances with chemical structures that permit no strong initial impression of safety and may even suggest a significant toxicity.	90 (1.5 µg/kg bw/day)

- For substances with genotoxic alerts, 0.15 µg/kg bw/day can be applied.
- For anticholinesterases (organic phosphates and carbamates), 0.3 µg/bw/day can be applied.
- In the calculations, TTC of 0.15 µg/kg bw/day has been applied for substances with non-genotoxic potential and CMR classification category 1A and 1B.
- Substances classified as CMR category 2 were assigned to Cramer class III with a TTC of 1.5 µg/kg bw/day.
- Substances with the remainder of hazard classifications including STOT SE were assigned to Cramer Class I with a TTC of 30 µg/kg bw/day.

The results of the calculations are given in Table 3. Calculated maximum acceptable concentrations for the two exposure scenarios, which are below the measured maximum concentration are highlighted in green. The calculated maximum concentrations are converted into more practical threshold values for the hotspot list by rounding off to 1-2 significant digits (see columns "HOTSPOT").

TABLE 3. Excerpt from Excel tool showing maximum found migration in CPR and virgin polymers, parameters used for each substance, the resulting maximum acceptable concentration for baby body lotion and baby shampoo and gel, and the hotspot maximum acceptable migration. Fields marked in grey denote identified hotspot substances.

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
2,4-Dimethylheptane or isomer	2213-23-2	12		3,00E-02	0,0000595	CC I	151 260,50	1 337 647,06		
Bis(2-ethylhexyl) phthalate (DEHP)	117-81-7	40		0,05	0,05	TDI EFSA	300,00	2 653,00		
1,6-Hexanediol diacrylate (HDDA)	13048-33-4	0,4		2,1	0,0471	Oral DNEL	13 375,80	118 286,62		
1-Butoxy-2-propanol	5131-66-8	6		12,5	0,3	Oral DNEL	12 500,00	110 541,67		
1-Decanol	112-30-1	30		12,5	0,0433	Oral DNEL	86 605,08	765 877,60		
1-Hexadecanol	36653-82-4	60		55	0,01	Oral DNEL	1 650 000,00	14 591 500,00		
2,2,4,4,6,8,8-Heptamethylnonane	4390-04-9	4		3,00E-02	0,0281	CC I	320,28	2 832,38		
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB)	6846-50-0	7		5	0,07	Oral DNEL	21 428,57	189 500,00		
2,4-diaminoanisol	615-05-4	0,015		1,50E-04	0,2584	CCIV	0,17	1,54		
2.4-Diaminotoluene	95-80-7	0,006		0,001	0,237	Oral DNEL	1,27	11,19		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
2,4-Diethyl-9H-thioxanthen-9-one	82799-44-8	0,25		0,104	0,1	Oral DNEL	312,00	2 759,12		
2,4-Dimethyl-1-heptene or isomer	19549-87-2	3		3,00E-02	0,0093	CC1	967,74	8 558,06		
2,4-Di-tert-butylphenol	96-76-4	160	6	0,007	1	Oral DNEL	**2,10**	**18,57**	2	20
Butylated Hydroxytoluene	128-37-0	50		0,25	1	Oral DNEL	75,00	663,25		
2,6-di-tert-butyl-1,4-benzoquinon	719-22-2	50	2,5	0,0015	0,3295	CCIII	**1,37**	**12,08**	1	10
2-Ethylhexyl salicylate	118-60-5	7		2,4	1	Oral DNEL	720,00	6 367,20		
2-Ethylhexyl-4-(dimethylamino)benzoate	21245-02-3	0,28		6,7	1	Dermal DNEL	2 010,00	17 775,10		
Oxybenzone	131-57-7	7		2	0,1	Oral DNEL	6 000,00	53 060,00		
2-Isopropylthioxanthone (2-ITX)	5495-84-1	0,17		0,1	0,1	Oral DNEL	300,00	2 653,00		
o-Ansidine	90-04-0	0,6		0,00015	1	CCIV	**0,05**	**0,40**	0,05	0,5
2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	71868-10-5	0,04		0,05	0,9715	Oral DNEL	15,44	136,54		
2-Methylbenzophenone og/eller 4-methylbenzophenone	131-58-8	0,6		0,03	0,4029	CC1 Hvis benzophenone så CCIV	22,34	197,54		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
2-Phenyldodecane	2719-61-1	5		0,03	0,3023	CCI	29,77	263,28		
2-Propylheptanol	10042-59-8	16		0,75	0,0526	Oral DNEL	4 277,57	37 827,95		
3,3'-dichlorobenzidine	91-94-1	0,1		0,00015	0,9927	CCIV	**0,05**	0,40	0,05	
3,5,5-Trimethyl-2(5H)-furanone	50598-50-0	7		0,03	0,0915	CCI	98,36	869,84		
3,5-di-tert-butyl-4-hydroxyaceto-phenon	14035-33-7	0,7		0,03	0,8009	CCI	11,24	99,38		
3,5-di-tert-butyl-4-hydroxybenzal-dehyd	1620-98-0	5	0,5	0,03	0,9887	CC1	9,10	80,50		
3,5-di-tert-butyl-4-hydroxystyren	52858-87-4	0,7	0,8	0,03	0,0061	CC1	1 475,41	13 047,54		
3-methyl-3,5-di-tert-butyl-4-hydro-xyphenylpropanoate	6386-38-5	0,8	12	0,03	0,9787	CC1	9,20	81,32		
Methyl 3-(3,5-di-tert-butyl-4-hy-droxyphenyl)propionate	6386-38-5	14	3	0,03	1	CC1	**9,00**	79,59	10	
3-Methyltridecane	6418-41-3	4		0,03	0,000771	CC1	11 673,15	103 229,57		
4,4'-Diaminodiphenylmethane	101-77-9	0,6		0,00015	1	CCIV	**0,05**	**0,40**	0,05	0,5
4-butoxyphenol	122-94-1	0,08		0,03	0,5252	CCI	17,14	151,54		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
p-Chloroaniline	106-47-8	0,022		0,0015	0,125	CCIV	3,60	31,84		
4-Chloro-o-toluidine	95-69-2	0,04		0,0015	0,1027	CCIV	4,38	38,75		
4-ethylphenol	123-07-9	1,2		0,417	0,1226	Oral DNEL	1 020,39	9 023,66		
4-Methyloctane or isomer	2216-34-4	3		0,03	0,0000704	CCI	127 840,91	1 130 539,77		
4-Phenylbenzophenone	2128-93-0	2,8		0,33	1	Oral DNEL	99,00	875,49		
4-Phenyldodecane	2719-64-4	5		0,03	0,0974	CC1	92,40	817,15		
4-Phenyltridecane	4534-51-4	4		0,03	0,1901	CC1	47,34	418,67		
4-tertbutylphenol	98-54-4	0,12	0,29	0,026	1	Oral DNEL	7,80	68,98		
5-Phenyldodecane	2719-63-3	2,7		0,03	0,0974	CC1	92,40	817,15		
5-Phenyltridecane	4534-50-3	4		0,03	0,1901	CC1	47,34	418,67		
6-Phenyltridecane	4534-49-0	4		0,03	0,1901	CC1	47,34	418,67		
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	310	20	0,03	0,9394	CC1	**9,58**	**84,72**	10	90

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
Acenaphten	83-32-9	0,5		0,03	0,3559	CC1	25,29	223,63		
Acetophenon	98-86-2	0,22		3,1	1	Oral DNEL	930,00	8 224,30		
Alifatic aldehyde, could be undecanal	112-44-7	3,1		1,65	1	Dermal DNEL (workers)	495,00	4 377,45		
Aluminium	7429-90-5	0,6		3,95	1	Oral DNEL	1 185,00	10 479,35		
Anthracen	120-12-7	1,7		1,2	1	Dermal DNEL (workers)	360,00	3 183,60		
Barium	7440-39-3	0,29		0,021	1	TDI (Drinking water)	6,30	55,71		
Benzoguanamine	91-76-9	0,6		0,096	0,75	Oral DNEL	38,40	339,58		
Benzophenone	119-61-9	2,2		0,05	0,7	Oral DNEL	21,43	189,50		
Benzyl Benzoate	120-51-4	6		1,42	0,7	Oral DNEL	608,57	5 381,80		
Benzylbutylphthalate	85-68-7	0,4		0,5	0,05	Oral DNEL	3 000,00	26 530,00		
Bumetrizole	3896-11-5	30		0,03	0,9897	CC1	**9,09**	80,42	10	
Calcium	7440-70-2	4		0,03	1	CC1	9,00	79,59		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
Co-elution, alifatic alcohol and eicosane (C20)	112-95-8	400	1100	0,03	0,139	CC1	64,75	572,59		
Eicosane	112-95-8	900	1100	0,03	1	CC1	9,00	79,6		
α-Hexylcinnamaldehyde	101-86-0	23		0,03	0,1446	CC1	**62,24**	550,41		
Tributyl acetylcitrate	77-90-7	5		0,5	1	Oral DNEL	150,00	1 326,50		
Decane, 2,3,5,8-tetramethyl-	192823-15-7	6		0,03	0,1	CC1	90,00	795,90		
Decene	872-05-9	6	9	0,03	0,0000504	CC1	178 571,43	1 579 166,67		
Dibutyl sebaccate	109-43-3	0,6		0,03	0,2282	CC1	39,44	348,77		
Dibutylphthalate	84-74-2	8		0,007	0,05	Oral DNEL	42,00	371,42		
Diethyl Phthalate	84-66-2	40		0,75	0,5	Oral DNEL	450,00	3 979,50		
Diisobutylphthalate	84-69-5	7	1	0,21	0,0921	Oral DNEL	684,04	6 049,19		
Dodecanoic acid, dodecyl ester	13945-76-1	80		0,03	0,7891	CC1	**11,41**	100,86	10	
Ester of benzoic acid, may be benzoic acid, undecyl ester	6316-30-9	8		0,03	0,3556	CC1	25,31	223,82		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
Ethyl 4-dimethylaminobenzoate	10287-53-3	0,08		0,15	1	Dermal DNEL (workers)	45,00	397,95		
Ethyl Oleate	111-62-6	24		0,03	0,3764	CC1	**23,91**	211,45		
Ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate	84434-11-7	0,016		0,5	1	Oral DNEL	150,00	1 326,50		
Fluoranthen	206-44-0	1,6		0,0015	0,9732	CCIV	**0,46**	4,09	0,5	
Fluoren	86-73-7	0,8		0,0015	0,7039	CCIII	**0,64**	5,65	0,6	6
Hexadecanoic acid, decyl ester	42232-27-9	22		0,03	0,812	CC1	**11,08**	98,02	10	
Hexadecanoic acid, dodecyl ester	42232-29-1	40		0,03	0,8223	CC1	**10,94**	96,79	10	
Hexadecanoic acid, methyl ester	112-39-0	21		0,03	0,105	CC1	85,71	758,00		
Isophorone	78-59-1	4		0,5125	0,0281	Oral DNEL	5 471,53	48 386,57		
Isopropyl myristate	110-27-0	40		1,6	0,0661	Oral DNEL	7 261,72	64 217,85		
Isopropyl palmitate	142-91-6	50		1,83	0,1811	Oral DNEL	3 031,47	26 808,34		
Jern	7439-89-6	0,28		0,71	1	Oral DNEL	213,00	1 883,63		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
Kalium	7440-09-7	1,2		0,03	1	CC1	9,00	79,59		
Kobber	7440-50-8	0,05		0,041	0,001106	Oral DNEL	11 121,16	98 348,10		
Limonene	138-86-3	24		0,03	0,000356	CC1	25 280,90	223 567,42		
Magnesium	7439-95-4	0,4		3,6	1	Oral DNEL	1 080,00	9 550,80		
Mangan	7439-96-5	0,011		0,0021	1	Dermal DNEL	0,63	5,57		
Methyl (3-oxo-2-pentylcyclopentyl)acetate (hedione)	24851-98-7	9		2,5	0,459	Oral DNEL	1 633,99	14 449,89		
Methyl dihydrojasmonate	24851-98-7	5		2,5	0,459	Oral DNEL	1 633,99	14 449,89		
Methyl elaidate (double bond may be different position)	112-62-9	14		0,03	0,2725	CC1	33,03	292,07		
Methyl stearate	112-61-8	7		6,95	0,4983	Oral DNEL	4 184,23	37 002,51		
Methyl-2-benzoylbenzoate (MBB)	606-28-0	0,4		0,052	0,9085	Oral DNEL	17,17	151,85		
Naphthalen	91-20-3	4		0,0015	0,0723	CCIII	6,22	55,04		
Natrium	7440-23-5	7		0,03	1	CC1	9,00	79,59		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
n-Hexyl salicylate	6259-76-3	40		0,3	0,078	Oral DNEL	1 153,85	10 203,85		
tert-Butyl cyclohexyl acetate	88-41-5	11		0,0015	0,0083	CCIII	54,22	479,46		
n-Propyl 11-octadecenoate	1000336-71-7	20		0,03	0,4956	CC1	**18,16**	160,59	20	
Octadecenamide or isomer	301-02-0	18		0,03	0,9881	CC1	**9,11**	80,55	10	
Octadecenoic acid ethyl ester	6114-18-7	4		0,03	0,3764	CC1	23,91	211,45		
Octan-2-yl palmitate	55194-81-5	22		0,03	0,667	CC1	**13,49**	119,33		
Octane	111-65-9	40		699	1	Dermal DNEL	209 700,00	1 854 447,00		
Octanoic acid, dodecyl ester	20292-09-5	8		0,03	0,4079	CC1	22,06	195,12		
Octinoxate	5466-77-3	60		0,0015	0,8622	CCIII	**0,52**	**4,62**	0,5	5
Octocrylene	6197-30-4	23		0,3825	0,002	Oral DNEL	57 375,00	507 386,25		
Octyl ether	629-82-3	17		25	0,005	Oral DNEL	1 500 000,00	13 265 000,00		
o-Cymene (or isomer)	527-84-4	7		0,03	0,000766	CC1	11 749,35	103 903,39		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
o-Toluidin	95-53-4	0,5		0,00015	0,0434	CCIV	1,04	9,17		
Pentacosane (C25)	629-99-2	12		0,03	0,6551	CC1	13,74	121,49		
Phenanthren	85-01-8	6		0,0015	0,9177	CCIII	**0,49**	**4,34**	0,5	5
Piperonyl butoxide	51-03-6	2,8		0,221	0,021	Oral DNEL	3 157,14	27 919,67		
Pyren	129-00-0	0,9		0,0015	0,9894	CCIIII	**0,45**	4,02	0,5	
Salicyclic acid	69-72-7	0,21		1	0,6	Oral DNEL	500,00	4 421,67		
Squalene	111-02-4	8		1,94	0,7893	Oral DNEL	737,36	6 520,74		
Strontium	7440-24-6	0,07		0,396	0,001	Oral DNEL	118 800,00	1 050 588,00		
Tetradecanoic acid, dodecyl ester	2040-64-4	50		0,03	0,812	CC1	**11,08**	98,02	10	
Tetraethylene glycol di-2-ethylhexoate	18268-70-7	7		0,523	0,1	Oral DNEL	1 569,00	13 875,19		
Tri(propylene glycol) diacrylate	42978-66-5	0,14		0,85	1	Dermal DNEL (workers)	255,00	2 255,05		
Tributyl citrate	77-94-1	0,21		12,5	1	Oral DNEL	3 750,00	33 162,50		

Component				CALCULATIONS					HOTSPOT Max. Conc. (mg/kg)	
	CAS no.	Max conc. (mg/kg)	Max conc. i virgin polymer (mg/kg)	DNEL/TDI/ Cramer Class mg/kg bw day	Dermal abs.	Choice of DNEL/TDI/Cramer Class	Baby body lotion Max Conc (mg/kg)	Baby shampoo and gel Max Conc (mg/kg)	Leave-on	Rinse-off
Tridecane (C13)	629-50-5	12		0,03	0,000947	CC1	9 503,70	84 044,35		
Trimethylolpropane triacrylate	15625-89-5	0,025		0,03	0,3934	CC1	22,88	202,31		
Tris-(2,4-di-t-butylphenyl) phosphite	31570-04-4	1000	150	0,6	0,801	Oral DNEL	**224,72**	1 987,27	225	
Undecane (C11)	1120-21-4	5		0,03	0,000151	CC1	59 602,65	527 086,09		
Versalide	88-29-9	21		0,03	0,2865	CC1	31,41	277,80		
Zink	7440-66-6	0,18		0,83	1	Oral DNEL	249,00	2 201,99		
α-Pinene	80-56-8	6		0,225	0,0000895	Oral DNEL	754 189,94	6 669 553,07		
4,4'-diaminodiphenylmethan	101-77-9	0,026		0,00021	1	Dermal DNEL (workers)	0,06	0,56		

An excel version of the data in Table 3 is found here:
https://mst.dk/media/256347/risk-analysis_recycled-plast.xlsm
Here, all the background data for the calculations are also included.

It could be discussed whether substances such as ethyl oleate and octan-2-yl palmitate should remain on the hotspot list. These are derivatives of the well-known fatty acids oleic acid and palmitic acid, and they do not appear on any of the hazard listings considered. Likewise, aliphatic alcohol and eicosane (C20) are common ingredients in cosmetics with no apparent toxicity. However, since no toxicological data could be readily found for these four substances, they were assigned a Cramer classification leading to a TTC of 0.03 mg/kg bw/day. The maximum concentrations found are larger than the acceptable concentrations calculated as a result of the TTC, but since no specific toxicological effects can be expected and that they are derivatives of relatively innocuous substances, we see no reason to justify their inclusion on a hotspot list. They are therefore removed from the two hotspot lists.

The total number of hotspot substances found by the risk-based method is the following:

- Leave-on hotspot list: 20 substances
- Rinse-off hotspot list: 7 substances

5.4 Selection of sensitising hotspot substances

In the previous sections, the selection of problematic substances for the hotspot list was based on a risk-based analysis. In this section, we would like to focus on sensitising substances. The risk-based analysis is less useful here because the sensitising mode of action is not systemic, but occurs locally, and does not necessarily require complete absorption through the skin.

Two groups of substances are considered in the following:

- substances, which are classified as skin sensitisers in the list of harmonised classification (HAR) or in the advisory list for self-classification (ADV)
- substances belonging to the group of fragrances. Focus is on the group of 26 **declarable** perfume substances or which is under consideration regarding declaration under the auspices of amendments to the Cosmetics Regulation (see more details in Table 1).

In figure 3 the result of an analysis with this focus is shown with the excel tool on substances in the reduced migration dataset. Substances are flagged with red and grey boxes, and are either classified as sensitisers (all are Skin Sens 1) or included on the total list of fragrances tabled in the SCCS report (2012)

Substances classified as sensitisers

Using the reporting threshold of 1000 ppb (= 1mg/kg) for sensitisers categorized as 1/1B in The Cosmetics Europe Advisory Report from 2019 (see also chapter 2.1 for further details), most of the substances highlighted with a red box in the Allergy column of Figure 3 would need to be reported. Including all of these substances, however, does not meet the goal of collecting a ***limited*** number of substances in the hotspot list.

A special case exists for the C12-C34 alkenes migrating from the samples, which we earlier decided not to include in the reduced migration dataset because their migration was observed originating both in PCR but also in virgin PE. These alkenes are on the Danish EPA advisory classification list, which is the result of QSAR estimations. However, upon a short search in the literature in PubMed, no cases of skin sensitisation to such substances are readily available. We therefore consider it doubtful whether these long-chain alkenes constitute a real hazard, and therefore conclude that the decision on not including them on the reduced migration dataset seems reasonable. This may be subject to further investigations.

Component	CASnr.	Max konc.	Max konc. i virgin polymer	Problematic substances		Classification	
				Allergy (class.)	Fragrances	HAR	ADV
2,4-Diaminotoluene	95-80-7	0,11				Carc. 1B; Muta. 2; Repr. 2; Acute Tox. 3 *; Acute Tox. 4 *; STOT RE 2 *; Skin Sens. 1; Aquatic Chronic 2;	
Butylated Hydroxytoluene	128-37-0	50					Muta. 2; Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2; Aquatic Acute 1; Aquatic Chronic 1
2,6-di-tert-butyl-1,4-benzoquinon	719-22-2	50	2,5				Repr. 2; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1
2-Propylheptanol	10042-59-8	16					Skin Sens. 1
3,3'-dichlorobenzidine	91-94-1	0,1				Carc. 1B; Acute Tox. 4 *; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1;	
4,4'-Diaminodiphenylmethane	101-77-9	0,6				Carc. 1B; Muta. 2; STOT SE 1; STOT RE 2 *; Skin Sens. 1; Aquatic Chronic 2;	
p-Chloroaniline	106-47-8	0,022				Carc. 1B; Acute Tox. 3 *; Acute Tox. 3 *; Acute Tox. 3 *; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1;	
4-ethylphenol	123-07-9	1,2					Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2
Alifatic aldehyde, could be undecanal	112-44-7	3,1					Skin Sens. 1; Aquatic Acute 1
α-Hexylcinnamaldehyde	101-86-0	270					Skin Sens. 1; Skin Irrit. 2; Aquatic Acute 1; Aquatic Chronic 1
Limonene	138-86-3	24				Flam. Liq. 3; Skin Irrit. 2; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1;	
Octyl ether	629-82-3	17					Skin Sens. 1
Squalene	111-02-4	8					Skin Sens. 1
Tri(propylene glycol) diacrylate	42978-66-5	230				STOT SE 3; Skin Irrit. 2; Eye Irrit. 2; Skin Sens. 1; Aquatic Chronic 2;	
Trimethylolpropane triacrylate	15625-89-5	140				Skin Irrit. 2; Eye Irrit. 2; Skin Sens. 1;	
α-Pinene	80-56-8	6					Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1
4,4'-diaminodiphenylmethan	101-77-9	0,026				Carc. 1B; Muta. 2; STOT SE 1; STOT RE 2 *; Skin Sens. 1; Aquatic Chronic 2;	
Benzyl Benzoate	120-51-4	6				Acute Tox. 4 *; Aquatic Chronic 2;	
Methyl (3-oxo-2-pentylcyclopentyl)acetate (hedione)	24851-98-7	9					
Methyl dihydrojasmonate	24851-98-7	5					
n-Hexyl salicylate	6259-76-3	40					Aquatic Acute 1; Aquatic Chronic 1

FIGURE 3. List of substances, which are either classified as sensitising or included on the fragrance list (SCCS, 2012) (ref. SCCS, 2012). Substances classified as sensitising can either be part of the harmonized or the advisory list respectively flagged with a dark or a light red box. Fragrances can either be part of the original 26 declarable, under consideration regarding declaration or on the residual list of fragrances flagged respectively with dark red, light red or grey boxes

Sensitising fragrance substances

Instead of focusing on *all* the substances classified as sensitisers, we would like to focus on the *specific* group of fragrances many of which also have sensitising properties.

Figure 3 includes four fragrance substances belonging to the group of declarable substances or the group of fragrances under consideration regarding declaration (see Table 1 for more details of these groups):

- Limonene (declarable)
- α-Pinene (under considerations for declaration)
- α-Hexylcinnamaldehyde (declarable)
- Benzyl Benzoate (declarable)

The concentration limits for when perfume substances must be declared in cosmetics are the following:

f. Leave-on products: 0,001% (10 mg/kg)
g. Rinse-off products: 0,01 % (100 mg/kg)

We have therefore added these four perfume substances to the hotspot lists for leave-on and rinse-off products with these concentration limits.

5.5 Other considerations

Finally, we would like to raise the question whether there are important categories of hazardous substances, which were not identified in the preceding chapters, but should be considered for the hotspot list.

Phthalates
No phthalates were identified as a problematic substance in the risk-based selection above. However, phthalates are known to be problematic, and in the Environmental Project no. 2174, the migration of phthalates were found to be a safety concern for baby body lotion, when the weighted concentration of DEHP equivalents were above ≈ 150 mg/kg (0,015%). We have therefore included a selection of phthalates on the hotspot list for leave-on products with a maximum weighted concentration limit of 150 mg/kg.

CMR; PAA and PAH substances
According to article 15 in the Cosmetics Regulation, CMR-substances are prohibited in cosmetic products.

Primary aromatic amines (PAA's) as a group could also be denoted as hotspot substances, since we do not have DNELs or TDIs for them, and they're illegal when found as migrants from plastic food contact materials. Presumably, they're all carcinogenic.

Polycyclic aromatic hydrocarbons (PAHs) as a group (including pyrene, fluoranthene, fluorene and naphthalene found in the analyses) could furthermore be denoted as hotspot substances, since they are regarded as no-threshold carcinogens, also in contact with skin.

The migration dataset contains members of all three of the above group of substances, not all of which were identified as hotspot substances in the preceding chapters. For all three groups, there are however many more members of the group, than what can in practice be analysed for. So even if we expanded the hotspot list with the additional CMR, PAA and PAH substances found in the migration dataset, it would still not be complete.

Also, as highlighted earlier, the lists of hotspot substances are not meant to be exhaustive and does not alleviate the user of performing proper safety assessments of all other migrating substances and conforming to other regulations such as 1) avoid CMR in cosmetics products 2) restrictions on PAA and PAH. Conforming to these regulations are the responsibility of the responsible person for the cosmetic product, whereas the hotspot documentation is intended to be used solely in the supply chain communication dealing with the PCR quality.

We have therefore decided not to include any additional CMR, PAA and PAH substances in the hotspot lists.

5.6 Resulting hotspot lists

The hotspot lists for the two areas: Use of recycled plastic respectively for Leave-on or Rinse-off packaging of cosmetics products is included in Table 4. The number of substances included in the two lists are:

- Leave-on: 28
- Rinse-off: 11

The migration analysis for the substances included in these two lists should document that the concentration is below the maximum concentration given here.

TABLE 4. Hotspot list for leave-on and rinse-off recycled plastics for packaging of cosmetics products.

Component	CAS nr.	HOTSPOT Max. Conc. (mg/kg)		Comments
		Leave-on	Rinse-off	
2,4-Di-tert-butylphenol	96-76-4	2	20	**RISK-BASED SUBSTANCES** This section list the hotspot substances identified by the risk-based method (chapters 5.1-5.3). From this result, four substances were removed from the list as discussed in chapter 5.3. - Ethyl oleate - Octan-2-yl palmitate - aliphatic alcohol - Eicosane (C20) since they are judged to be relatively innocuous substances
2,6-di-tert-butyl-1,4-benzoquinon	719-22-2	1	10	
o-Ansidine	90-04-0	0,05	0,5	
3,3'-dichlorobenzidine	91-94-1	0,05		
Methyl 3-(3,5-di-tert-butyl-4-hydroxy-phenyl)propionate	6386-38-5	10		
4,4'-Diaminodiphenylmethane	101-77-9	0,05	0,5	
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	10	90	
Bumetrizole	3896-11-5	10		
Dodecanoic acid, dodecyl ester	13945-76-1	10		
Fluoranthen	206-44-0	0,5		
Fluoren	86-73-7	0,6		
Hexadecanoic acid, decyl ester	42232-27-9	10		
Hexadecanoic acid, dodecyl ester	42232-29-1	10		
n-Propyl 11-octadecenoate	1000336-71-7	20		
Octadecenamide or isomer	301-02-0	10		
Octinoxate	5466-77-3	0,5	5	
Phenanthren	85-01-8	0,5	5	
Pyren	129-00-0	0,5		
Tetradecanoic acid, dodecyl ester	2040-64-4	10		
Tris-(2,4-di-t-butylphenyl) phosphite	31570-04-4	225		
Bis(2-ethylhexyl) phthalate (DEHP)	117-81-7	150		**PHTHALATES SUBSTANCES** Concentration limit is a weighted total concentration of the four phthalates DEHP, DIBP, DBP and BBP.
Diisobutylphthalate (DIBP)	84-69-5			
Dibutylphthalate (DBP)	84-74-2			
Benzyl Butylphthalate (BBP)	85-68-7			
Limonene	138-86-3	10	100	**FRAGRANCE SUBSTANCES**
α-Hexylcinnamaldehyde	101-86-0	10	100	
Benzyl Benzoate	120-51-4	10	100	
α-Pinene	80-56-8	10	100	

5.7 Discussion

The hotspot list is created mainly with worst case exposures of babies in mind, comparing the maximum concentrations found in PCR samples in Environmental Project no. 2174. We have checked whether any of the samples analyzed could have passed the leave-on hotspot list as created here. The answer is no. In the initial safety assessment, all but one sample was found to contain problematic substances to an unacceptable extent. The last sample will fall on the content of α-hexylcinnamaldehyde, a perfume substance. This emphasizes the need to be careful about selecting the sources of PCR, since perfume contamination seems to be limiting.

The fact that the PCR samples evaluated in this project all failed the leave-on hotspot list does not mean that there is no chance some other samples could meet the criteria in the leave-on hotspot list. Industry is presently working at improving the process for recycling the plastic, and the developed set of hotspot substances might also guide these developments to develop higher quality PCR plastic. The rinse-off hotspot list is easier to pass, and hence a few of the PCR samples might be used for rinse-off cosmetics.

Finally, our risk assessment, as in the initial project, is based on small packages. It should be borne in mind that dilution may solve some of the problems: Dilution by only using a fraction of PCR in the plastic packaging material; or dilution by using PCR for containers holding large volumes of product and/or smaller thickness of the container.

6. Total migration as criteria for PCR quality

The primary focus for the activities in this project is to develop hotspot lists of hazardous substances, which should be documented not to be contained in PCR recyclates.

In addition to the specific hotspot criteria, a total migration limit could also be considered. Plastic for food contact must always be tested for total migration, where the limit is 60 ppm for the total amount of migrants. In the following, we will discuss a basis for the introduction of a total migration limit in the PCR documentation. The discussion will mainly be based on data from the comparison between migration from virgin and PCR PE samples.

Table 5 lists substances, which were not identified in the migration dataset as matching any of the hazard lists. The table compares the maximum migration found in PCR with the maximum migration found in the virgin PE samples.

It is clear from this table that the alkanes are found migrating at around the same level from PCR and virgin PE. The three substances marked in green seem to migrate from PCR in considerably higher amounts than from virgin PE. Of these, 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione (CAS no 82304-66-3) deserves a little more attention because of the maximum migration of 310 mg/kg.

TABLE 5. Comparison of maximum migration from PCR of substances, which could not be matched with any hazard list with the maximum migration found in the virgin PE samples.

Analysis Method	CAS	Substance name	Max conc. mg/kg	
			PCR	Virgin
PE-phenols	1620-98-0	3,5-di-tert-butyl-4-hydroxybenzaldehyd	5	0.5
PE-phenols	52858-87-4	3,5-di-tert-butyl-4-hydroxystyren	0.8	0.8
PE-phenols	6386-38-5	3-methyl-3,5-di-tert-butyl-4-hydroxyphenylpropanoate	0.8	12
GC-MS	6386-38-5	Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	14	3
GC-MS	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	310	2.7
PE-phenols	82304-66-3	7,9-di-tert-butyl-1-oxaspiro(4,5)decra-6,9-diene-2,8-dione	26	20
GC-MS	593-45-3	Co-elution, Octadecane (C18) and unsaturated alkane	900	900
GC-MS	593-45-3	Octadecane (C18)	900	900
GC-MS	629-97-0	Docosane (C22)	900	1300
GC-MS	112-40-3	Dodecane (C12)	500	240
GC-MS	544-85-4	Dotriacontane (C32)	40	50
GC-MS	630-01-3	Hexacosane (C26)	700	1200
GC-MS	544-76-3	Hexadecane (C16)	800	900

Analysis Method	CAS	Substance name	Max conc. mg/kg	
			PCR	Virgin
GC-MS	630-02-4	Octacosane (C28)	500	800
GC-MS	646-31-1	Tetracosane (C24)	800	1200
GC-MS	629-59-4	Tetradecane (C14)	700	700
GC-MS	638-68-6	Triacontane (C30)	230	240

To solve the problem of dealing with the migration of many toxicologically unknown and non-intentionally added substances, it might be fair to have a total migration limit for PCR in line for what is required for plastic food contact materials. For plastic food contact materials, the total migration limit is 60 mg/kg food. In Environmental Project no. 2174 we calculated that a TDI value of 10 mg/kg bw/day would result in a maximum allowable concentration of 3000 mg/kg cosmetic product. With this calculation as a point of departure, a total migration limit could be suggested to be 3000 mg/kg cosmetic product.

The total migration limit of 3000 mg/kg cosmetic product or simulant should be understood as the total count of all migrants added up. Substances with a lower TDI value than 10 mg/kg bw/day should still be subject to the corresponding lower acceptable concentration but be included in the total migration.

From table 6 below, it appears that not all virgin PE samples would be below the total migration limit. Here it is only one out of three, and for the PCR-samples, it was three out of seven.

TABLE 6. Comparison of total migration and number of detected components in virgin and PCR PE

Sample	Plastic source	Total amount detected, [naphthalene equivalent mg/kg]	Number of detected components	Green: results below suggested total migration limit
970130-1**	Virgin	9400	65	
970130-2**	Virgin	640	17	
970130-3**	Virgin	4700	66	
1.1***	PCR PE	2100	41	
2.1***	PCR PE	7700	48	
3.3***	PCR PE	4000	69	
3.5***	PCR PE	3700	95	
4.2***	PCR PE	2300	57	
5.3***	PCR PE	5700	116	
5.4***	PCR PE	980	30	

**: Samples and results from DTI report 970130 rev.1. (see appendix 2) and private communication
***: Samples and results from (Danish Technological Institute and DHI A/S, 2021).

The product simulant used for PCR-PE resin was 95%-ethanol, and for virgin PE resin there was used isooctane (both 3 days at 60°C) with the proposed total migration criterion of 3000 mg/kg cosmetic product.

Since it was not possible to differentiate between total migration for virgin and PCR PE, we do not recommend that this criterion is included in the proposal for a PCR documentation at this time. The option could be considered in later revisions.

7. Conclusion

We have developed two hotspot lists for PCR to be used for packaging of cosmetics: One for leave-on products and one for rinse-off products. The hotspot list for leave-on products comprises 28 substances or substance groups, whereas the hotspot list for rinse-off products comprises 11 substances.

The main components on the lists have been developed by a risk-based screening method. Additional substances have been added based on evaluation of sensitising substances and considerations regarding the phthalates group.

As part of the work, an excel screening tool have been developed. The excel screening tool may be used as an aid to deal with the multitude of substances often being the result of migration analyses of PCR.

A total migration limit corresponding to what is required for plastic food contact materials have been considered but has not been included in this first version of our recommendation for hotspot lists.

The hotspot lists are thought of as a tool to document whether a limited number of problematic substances will be migrating from a PCR sample. We suggest that this documentation can then be used in the supply chain communication relating to the PCR quality. However, it does not relieve manufacturers of cosmetic products of the duty to perform safety assessments of the packaging containing PCR and conforming to other regulation.

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9. Appendices

Appendix 1. Results of literature search

A search for additional guidance documents in PubMed, Google Scholar and Science Direct was carried out.

Search terms	Limitation	No of hits	Remarks
Recycled plastic/PubMed		3479	
	AND post consumer	199	
	AND post consumer safety	83	Predominantly safety assessments from EFSA concerning recycling processes of PET
Recycled plastic/Google Scholar		544.000	
	AND post consumer	61.600	
	AND post consumer safety	52.900	
Recycled plastic post consumer safety cosmetic packaging/Google Scholar	Since 2020	12.400	No further guidance found
Recycled plastic post consumer safety cosmetic packaging/Science Direct	Since 2020	155	No further guidance found

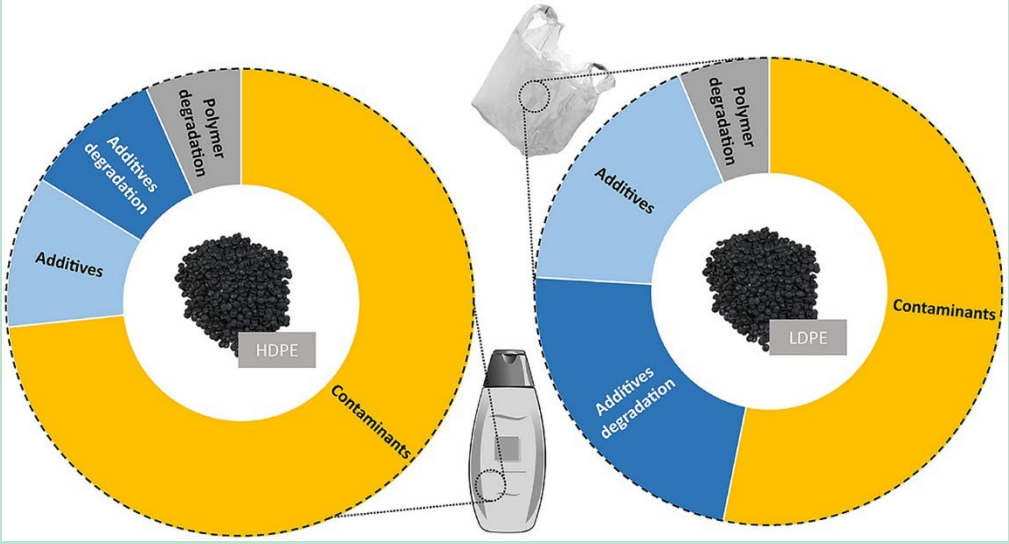
The following publications of interest were identified:

O. Horodytska, A. Cabanes, A. Fullana. Non-intentionally added substances (NIAS) in recycled plastics, Chemosphere, Volume 251, 2020,126373,ISSN 0045-6535, https://doi.org/10.1016/j.chemosphere.2020.126373. (https://www.sciencedirect.com/science/article/pii/S004565352030566X)

Abstract
The demand for high quality recycled polymers in the European plastic industry is on the increase, likely due to the EU's Plastic Strategy intended to implement the circular economy model in this sector. The problem is that there is not enough recycled plastic in the market. In terms of volume, post-consumer plastic waste could be key to meet the current and future demand. Nevertheless, a high level of contamination originated during the product's life cycle restricts its use. The first step to change this must be identifying the undesired substances in post-consumer plastics and performing an effective risk assessment. The acquired knowledge

will be fundamental for the development of innovative decontamination technologies. In this study, 134 substances including volatile and semi-volatile compounds have been identified in recycled LDPE and HDPE from domestic waste. Headspace and solvent extraction followed by GC/MS were used. The possible origin of each substance was studied. The main groups were additives, polymer and additives breakdown products, and contamination from external sources. The results suggest that recycled LDPE contains a broader number of additives and their degradation products. Some of them may cause safety concerns if reused in higher added value applications. Regarding recycled HDPE, the contaminants from the use phase are predominant creating problems such as intense odors. To reduce the number of undesired substances, it is proposed to narrow the variety of additives used in plastic manufacturing and to opt for separate waste collection systems to prevent cross-contamination with organic waste.
Keywords: Mechanical-recycling; Plastics; Domestic-waste; Polyolefins; NIAS; IAS

Illustration from the article: This shows the differences between recycled HDPE and recycled LDPE. Recycled LDPE contains a broader number of additives and their degradation products



López de Dicastillo C, Velásquez E, Rojas A, Guarda A, Galotto MJ. The use of nanoadditives within recycled polymers for food packaging: Properties, recyclability, and safety. Compr Rev Food Sci Food Saf. 2020 Jul;19(4):1760-1776. doi: 10.1111/1541-4337.12575. Epub 2020 May 31. PMID: 33337105.

Abstract
Nanotechnology is considered a highly valued technology to reduce the current environmental problem that is derived from plastic accumulation. The need to recycle and reuse packaging materials is essential to create a sustainable society towards a circular economy. However, the reprocessing of polymers leads to the deterioration of their characteristic mechanical, optical, thermal, and barrier properties due to the degradation of their polymeric chains. When recycled polymers are reinforced with nanoadditives, aforementioned properties improve and their use in the circular economy is more viable. In this review, different types of nanoadditives and recent advances in the development of recycled polymer nanocomposites reinforced with nanoadditives will be presented. In addition, there is a description of two research topics of current interest, recyclability of nanocomposites and safety for food packaging applications.

Recyclability of nanocomposites requires a study that includes the nature of the polymer matrix, the type of polymer and the concentration of nanofiller, the morphology, the presence of additives, and the conditions of the thermal-mechanical cycles. Finally, safety section is dedicated to clarify the migration process in nanoreinforced-recycled polymers in order to assess their safety for food contact applications.

Appendix 2. Analysis report

Analysis Report

REPORT NUMBER:
970130 rev.1
This analytical report replaces report 970130

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Assignor:	Danish Environmental Protection Agency Tolderlundsvej 5 DK-5000 Odense C
Item:	Analysis of virgin PE resin (MST ID nr.: 2641528)
Sampling:	The assignor
Period:	Samples received: 1 and 3 March 2021 Test performed: 3 March – 5 May 2021
Storage:	The test material will be destroyed after 3 months, unless otherwise agreed in writing.
Remark:	The account of the method(s) used only concerns the analysed sample(s).
Terms:	This test was conducted in accordance with international requirements (ISO/IEC 17025:2017) and in accordance with the General Terms and Conditions of Danish Technological Institute. The test results solely apply to the tested item(s) or to the sub-sample(s) selected for analysis. This analysis report may be quoted in extract only if Danish Technological Institute has granted its written consent.
Date/place:	26 August 2021 Danish Technological Institute, Aarhus Laboratory for Chemistry and Microbiology
Signature:	Søren Ryom Villadsen Senior Consultant Søren Ryom Villadsen 2021.08.26 12:40:31 +02'00'

Introduction

Three samples of virgin PE resin has been received for an accelerated migration study using the product simulant iso-octane. The iso-octane has then been analysed for the content of PAH and PE-phenols, and a general GC/MS screening has been performed.

This report follows a study performed previously and which has been presented in a a project report[1] authored by both Danish Technological Institute and Danish Environmental Protection Agency. The project report was focused on on migration from post-consumer recycled PE resin (PCR PE resin) to product simulants.

This report enables a comparison between the migration from virgin and PCR, and this comparison is delivered in a separate addendum to this report.

Sample marking

Laboratory label	Assignor label
970130-1	Polymer 1
970130-2	Polymer 2
970130-3	Polymer 3

Samples are provided by three different Danish companies producing cosmetics. It is informed that the samples are representative for polymer qualities that would normally be used for packaging material for cosmetics. The samples were made available through Danish Environmental Protection Agency and sent directly from producers to Danish Technological Institute. The producers and compounders of the samples are known by Danish Environmental Protection Agency and Danish Technological Institute. The knowledge is not disclosed in this report by request of Danish Environmental Protection Agency.

Packaging

Sample 970130-1 and 970130-2 were received in plastic bags. Sample 970130-3 was received in a closed container.

Figure 1: Pictures of the three samples as they were received. From left to right: 970130-1, 970130-2, 970130-3. White bars in pictures are edits for anonymisation of samples.

[1] "Initial safety assessment of recycled plastic for packaging of cosmetic products", Danish EPA, unreleased, DTI reference number 935492.

Analysis program

A migration at 60°C for a period of 3 days to the product simulant isooctane was performed. Pictures was taken before and after migration. The isooctane was subsequently analysed for the content of PE-phenols (degradation products of antioxidants and stabilizers), polyaromatic hydrocarbons (PAH) and screened by GC/MS screening procedure.

Analysis method

PE-phenols (degradation products of antioxidants and stabilisers)
A part of the product simulant (iso-octane) was taken and diluted 1:1 with dichloromethane with internal standards added. The extract was analysed by gas chromatography coupled with a mass selective detector (GC/MS). The identification of each component was identified by comparison of retention time and mass spectrum to the of reference standard. The quantification was performed using a calibration curve.

Detection limit: 0.1 – 1.5 mg/kg product simulant (see result table for compound specific detection limit)
Uncertainty: 15 % RSD

PAH (polycyclic aromatic hydrocarbons)
A part of the product simulant (iso-octane) was taken and diluted 1:1 with dichloromethane with internal standards added. The extract was analysed by gas chromatography coupled with a mass selective detector (GC/MS). The identification of each component was performed by comparison of retention time and mass spectrum to the of reference standard. The quantification was performed using a calibration curve.

Detection limit: 0.2 mg/kg product simulant (see result table for compound specific detection limit)
Uncertainty: 15 % RSD

GC/MS screening
A part of the product simulant (iso-octane) was taken and diluted 1:1 with dichloromethane with internal standards added. The extract was analysed by gas chromatography coupled with a mass selective detector (GC/MS). The identification of each component was performed using the NIST MS 2020 database and chemical evaluation. The quantification was performed semi-quantitatively and expressed naphthalene equivalents.

Detection limit: 3 mg/kg product simulant expressed as naphthalene equivalents
Uncertainty: Unknown

Results

Migration

Sample number	Product simulant	Sample amount [g]	Volume of simulant [mL]	Temperature [°C]	Migration period [days]
970130-1	Iso-octane	35	30	60	3
970130-2	Iso-octane	35	30	60	3
970130-3	Iso-octane	35	30	60	3

Figure 2: Picture of sample 970130-1 with product simulant (isooctane). The picture on the left is before the three-day migration and the picture on the right is after the migration. Note that no significant swelling is observed.

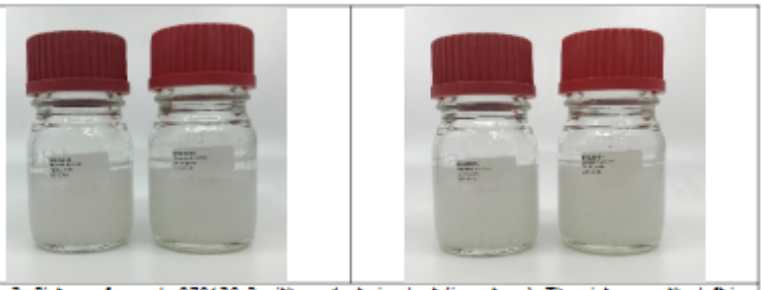


Figure 3: Picture of sample 970130-2 with product simulant (isooctane). The picture on the left is before the three-day migration and the picture on the right is after the migration. Note that no significant swelling is observed.

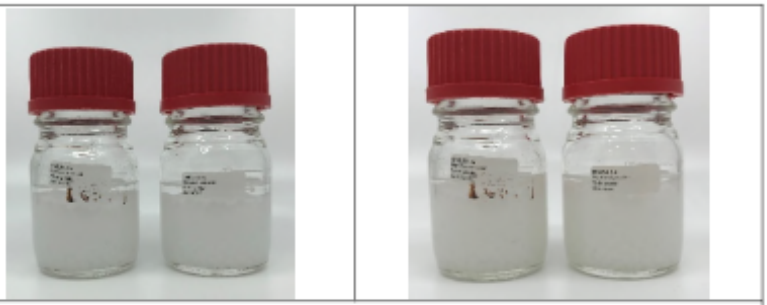


Figure 4: Picture of sample 970130-3 with product simulant (isooctane). The picture on the left is before the three-day migration and the picture on the right is after the migration. Note that no significant swelling is observed.

Figure 5: Picture of the simulant (iso-octane) after migration. A blank sample is seen to the left and going towards right, sample 970130-1, 970130-2 and to the far-right sample 970130-3. Sample 970130-1 and 970130-3 were cloudy after migration, see also figure 6.

Figure 6: Three pictures of simulant after migration from sample (to the right) in direct comparison to a blank simulant (to the left). From left to right is sample 970130-1, 970130-2 and 970130-3. The simulant from sample 970130-1 and 970130-3 appears cloudy.

PE-phenols migrated to iso-octane simulant

Component	CAS no.	970130-1# [mg/kg]	970130-2# [mg/kg]	970130-3# [mg/kg]	Detection limit# [mg/kg]
Acetophenone	98-86-2	-	-	-	0.2
5-Methyl-2-hexanone	110-12-3	-	-	-	1.5
4-Ethylphenol	123-07-9	-	-	-	0.2
4-tert-Butylphenol	98-54-4	-	-	0.29	0.1
4-Butoxyphenol	122-94-1	-	-	-	0.1
2,6-Di-tert-butyl-1,4-benzoquinone	719-22-2	2.5	-	0.95	0.8
2,4-Di-tert-butylphenol	96-76-4	-	-	-	0.8
2,6-Bis(1,1-dimethyl)-4-methylphenol	128-37-0	2.5	0.14	6.4	0.1
3,5-Di-tert-butyl-4-hydroxystyrene	52858-87-4	0.37	-	0.80	0.2
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0	0.53	0.20	0.20	0.2
3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	-	-	-	0.3
7,9-Di-tert-butyl-1-oxaspiro(4,5)decra-6,9-diene-2,8-dione	82304-66-3	17	0.47	20	0.2
3-Methyl-3,5-di-tert-butyl-4-hydroxyphenyl-propanoate	6386-38-5	4.6	1.7	12	0.2
3,5-Di-tert-butyl-4-hydroxybenzoic acid	1421-49-4	-	-	-	0.8
3,5-Di-tert-butyl-4-hydrophenyl propionic acid	20170-32-5	-	-	-	0.8

#: Expressed as mg component per kg product simulant
-: There was not observed a concentration above the detection limit

PAH compounds migrated to iso-octane simulant

Component	CAS no.	970130-1# [mg/kg]	970130-2# [mg/kg]	970130-3# [mg/kg]	Detection limit# [mg/kg]
Naphthalene	91-20-3	-	-	-	0.2
Acenaphtene	83-32-9	-	-	-	0.2
Acenaphtylene	208-96-8	-	-	-	0.2
Phenanthrene	85-01-8	-	-	-	0.2
Anthracene	120-12-7	-	-	-	0.2
Fluorene	86-73-7	-	-	-	0.2
Fluoranthene	206-44-0	-	-	-	0.2
Pyrene	129-00-0	-	-	-	0.2
Benzo(a)anthracene	56-55-3	-	-	-	0.2
Chrysene, triphenylene	218-01-9, 217-59-4	-	-	-	0.2
Benzo[b]fluoranthen Benzo[j]fluoranthen, Benzo[k]fluoranthen	205-99-2, 205-82-3, 207-08-9	-	-	-	0.2
Benzo(a)pyrene, Benzo(e)pyrene, Perylene	50-32-8, 192-97-2, 198-55-0	-	-	-	0.2
Indeno(1,2,3-cd)pyrene	193-39-5	-	-	-	0.2
Dibenzo[a,h]anthracene	200-181-8	-	-	-	0.2
Benzo[ghi]perylene	191-24-2	-	-	-	0.2

Multiple compounds and CAS no. for one result signifies, that the result is a sum of the given PAH
#: Expressed as mg component per kg product simulant
-: There was not observed a concentration above the detection limit

GC/MS screening of sample 970130-1

Component (970130-1)	RT [min]	CAS no.	Concentration* [mg/kg]
Decane	7.239	124-18-5	9.8
Dodecane	8.407	112-40-3	240
Saturated, branched alifatic compound (C12)	8.441	-	2.5
Saturated, branched alifatic compound (C14)	9.189	-	11
Saturated, branched alifatic compound (C14)	9.287	-	9.1
Tetradecane	9.441	629-59-4	660
Saturated, branched alifatic compound (C14)	9.512	-	11
Saturated, branched alifatic compound (C16)	10.172	-	7.8
Saturated, branched alifatic compound (C16)	10.206	-	15
Saturated, branched alifatic compound (C16)	10.320	-	13
Hexadecane	10.490	544-76-3	910
Not identified, unsaturated alifatic or alifatic alcohol	10.608	-	20
Saturated, branched alifatic compound (C16)	11.322	-	12
Not identified, likely saturated alifatic compound	11.371	-	17
Saturated, branched alifatic compound (C18)	11.516	-	14
Octadecane	11.725	593-45-3	940
Not identified, likely unsaturated alifatic compound (C18:1)	11.860	-	2.8
Not identified, could be octadecanol	11.904	(112-92-5)	20
Saturated, branched alifatic compound (C20)	12.685	-	5.8
Saturated, branched alifatic compound (C20)	12.709	-	11
Saturated, branched alifatic compound (C20)	12.773	-	20
Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	12.918	6386-38-5	3.2
Saturated, branched alifatic compound (C20)	12.952	-	17
Eicosane	13.200	112-95-8	1100
Not identified, unsaturated alifatic or alifatic alcohol	13.383	-	3.3
Not identified, unsaturated alifatic or alifatic alcohol	13.436	219750-68-2	24
Not identified, likely saturated, branched alifatic compound	14.044	-	3.7
Not identified, likely saturated, branched alifatic compound	14.267	-	11
Saturated, branched alifatic compound (C22)	14.303	-	9.3
Saturated, branched alifatic compound (C22)	14.379	-	21
Saturated, branched alifatic compound (C22)	14.580	-	17
Docosane	14.850	629-97-0	1300
Not identified, unsaturated alifatic or alifatic alcohol	15.071	-	2.6
Not identified, unsaturated alifatic or alifatic alcohol	15.126	-	28
Saturated, branched alifatic compound (C22)	15.692	-	5
Saturated, branched alifatic compound	15.935	-	15
Saturated, branched alifatic compound	15.980	-	8.7
Saturated, branched alifatic compound (C24)	16.059	-	22
Saturated, branched alifatic compound	16.265	-	17
Tetracosane	16.530	646-31-1	1200

Component (970130-1)	RT [min]	CAS no.	Concentration* [mg/kg]
Not identified	16.782	-	2.7
Not identified, may be unsaturated alifatic or alifatic alcohol	16.833	-	30
Saturated, branched alifatic compound (C26)	17.340	-	5.3
Co-elution, saturated, branched alifatic compound (C26) and not identified	17.561	-	15
Not identified, likely saturated, branched alifatic compound	17.620	-	5.8
Not identified, likely saturated, branched alifatic compound	17.700	-	21
Saturated, branched alifatic compound (C26)	17.900	-	15
Hexacosane	18.156	630-01-3	1210
Not identified, may be unsaturated alifatic or alifatic alcohol	18.470	-	28
Not identified	18.913	-	4
Saturated, branched alifatic compound (C28)	19.106	-	12
Saturated, branched alifatic compound (C28)	19.168	-	3.5
Saturated, branched alifatic compound	19.245	-	16
Saturated, branched alifatic compound (C28)	19.435	-	9.1
Octacosane	19.664	630-02-4	750
Saturated, branched alifatic compound	19.998	-	17
Saturated, branched alifatic compound (C30)	20.546	-	5.9
Saturated, branched alifatic compound (C30)	20.684	-	6.2
Saturated, branched alifatic compound (C30)	20.867	-	2.8
Triacontane	21.069	638-68-6	240
Not identified	21.458	998309-31-0	3.5
Dotriacontane	22.576	544-85-4	52
Tris-(2,4-di-t-butylphenyl) phosphite	24.186	31570-04-4	150
Saturated alifatic compound	24.392	-	15
Saturated alifatic compound	26.746	-	6.6

*: Expressed as mg component as naphthalene equivalent per kg product simulant

GC/MS screening of sample 970130-2

Component (970130-2)	RT [min]	CAS no.	Concentration* [mg/kg]
Decene (C10:1)	7.202	872-05-9	9.4
Dodecene (C12:1)	8.371	112-41-4	27
Tetradecene (C14:1)	9.409	1120-36-1	46
Hexadecene (C16:1)	10.455	629-73-2	63
Octadecene (C18:1)	11.684	112-88-9	76
Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	12.916	6386-38-5	4.7
Eicosene (C20:1)	13.153	3452-07-1	84
Not identified, may be unsaturated alifatic or alifatic alcohol	14.009	-	3.3
Docosene (C22:1)	14.797	1599-67-3	86
Tetracosene (C24:1)	16.482	10192-32-2	79
Hexacosene (C26:1)	18.106	18835-33-1	65
Octacosene (C28:1)	19.631	18835-34-2	45
Triacontene (C30:1)	21.054	18435-53-5	22
Dotriacontene (C32:1)	22.589	18435-55-7	6.3
2,6-Di-tert-butyl-4-[(2-octadecyloxycarbonyl)ethyl]phenol (irganox 1076)	27.220	2082-79-3	26

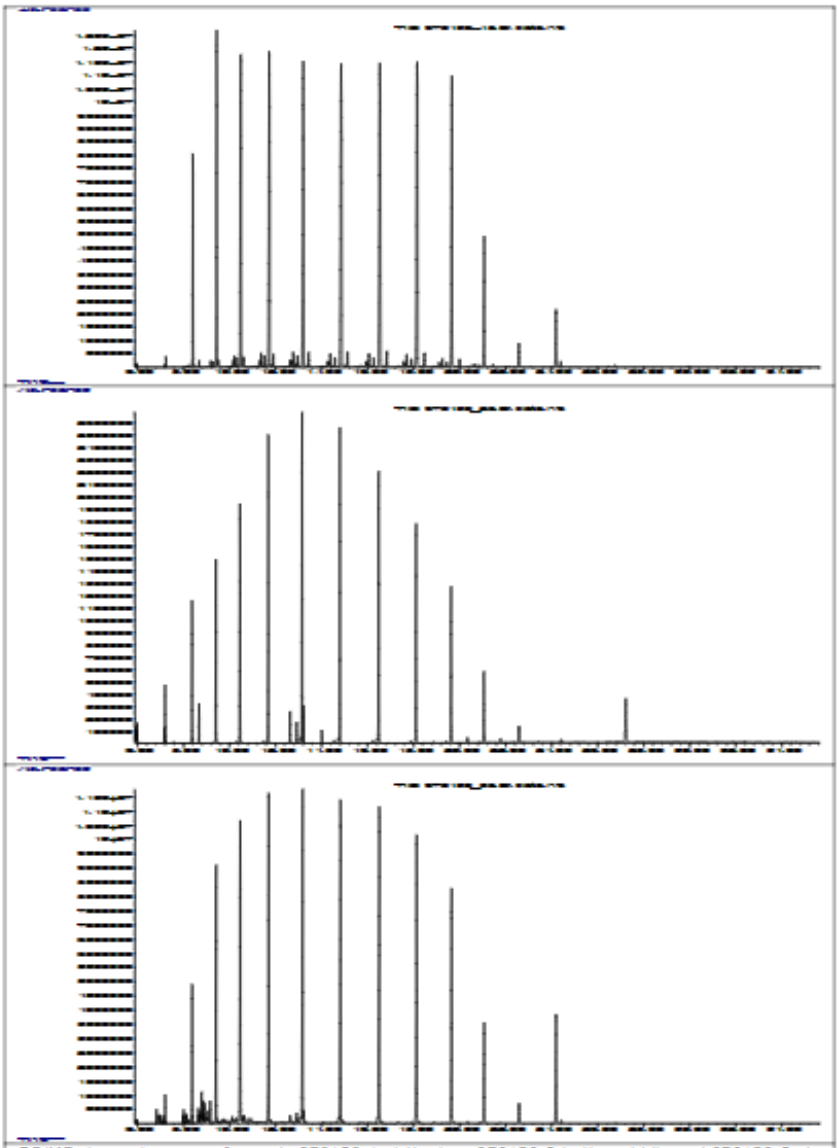
*: Expressed as mg component as naphthalene equivalent per kg product simulant

GC/MS screening of sample 970130-3

Component (970130-3)	RT [min]	CAS no.	Concentration* [mg/kg]
Not identified, likely saturated alifatic	6.824	-	10
Not identified, likely saturated, branched alifatic (C10)	6.937	-	5.7
Not identified, likely unsaturated, branched alifatic (C10)	6.956	-	6.2
Not identified, likely unsaturated, branched alifatic (C10)	7.044	-	2.6
Not identified, likely unsaturated, branched alifatic (C10)	7.124	-	5.3
Decene (C10:1)	7.206	872-05-9	21
Not identified, may be unsaturated, branched alifatic (C10) or alifatic alcohol	7.975	-	6.4
Not identified, may be unsaturated, branched alifatic (C10) or alifatic alcohol	8.003	-	11
Not identified, may be unsaturated, branched alifatic (C12) or alifatic alcohol	8.103	-	7.1
Not identified, may be unsaturated, branched alifatic (C12) or alifatic alcohol	8.127	-	8.2
Unsaturated, branched alifatic (C12)	8.171	-	2.8
Unsaturated, branched alifatic (C12)	8.260	-	5
Dodecene (C12:1)	8.375	112-41-4	130
Unsaturated, branched alifatic (C14)	8.645	-	20
Not identified, may be unsaturated, branched alifatic or alifatic alcohol	8.744	-	15
Not identified, may be unsaturated, branched alifatic or alifatic alcohol	8.784	-	43
Unsaturated, branched alifatic	8.840	-	8
Saturated, branched alifatic	8.873	-	21
Not identified, may be unsaturated, branched alifatic or alifatic alcohol	8.907	-	27
Unsaturated, branched alifatic (C14)	8.936	-	2.8
Not identified, like saturated, branched alifatic	8.999	-	3.5
Unsaturated, branched alifatic (C14)	9.028	-	6.6
Unsaturated, branched alifatic (C14)	9.068	-	22
Not identified, may be unsaturated, branched alifatic	9.162	-	30
Tetradecene (C14:1)	9.415	1120-36-1	300
Unsaturated, branched alifatic (C14)	9.470	-	2.5
Unsaturated alifatic (C14)	9.540	-	3.3
Not identified, alifatic compound	9.687	-	6
Not identified	9.752	-	6.7
Unsaturated, branched alifatic (C16)	9.880	-	4.2
Not identified, alifatic compound	10.075	-	3.5
2,4-Di-tert-butylphenol	10.119	96-76-4	6.4
Not identified, alifatic compound	10.150	-	3
Not identified, alifatic compound	10.235	-	4.5
Not identified, may be alifatic compound and possibly alcohol functionality	10.300	-	7.2
Hexadecene (C16:1)	10.465	629-73-2	440
Not identified, alifatic compound	10.593	-	7.7
Not identified, may be alifatic compound and possibly alcohol functionality	10.628	-	9.8

Component (970130-3)	RT [min]	CAS no.	Concentration* [mg/kg]
Not identified, may be alifatic compound and possibly alcohol functionality	10.790	-	10
Not identified, may be alifatic compound and possibly alcohol functionality	10.938	-	8.7
Not identified	11.343	-	2.6
Octadecene (C18:1)	11.701	112-88-9	470
Not identified, may be alifatic compound and possibly alcohol functionality	11.775	-	3.2
Not identified	12.570	-	2.8
Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	12.917	6386-38-5	11
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.964	82304-66-3	2.7
Not identified, alifatic compound	13.100	-	3.5
Eicosene (C20:1)	13.176	3452-07-1	530
Not identified, may be alifatic compound and possibly alcohol functionality	13.260	-	2.7
Not identified, may be alifatic compound and possibly alcohol functionality	14.743	-	6.9
Docosene (C22:1)	14.824	1599-67-3	580
Not identified, may be alifatic compound	14.915	-	3.1
Not identified, may be alifatic compound	15.683	-	2.9
Not identified, may be alifatic compound	16.432	-	3.6
Tetracosene (C24:1)	16.510	10192-32-2	570
Not identified, may be alifatic compound and possibly alcohol functionality	16.601	-	3.1
Not identified, may be alifatic compound and possibly alcohol functionality	17.321	-	3.6
Hexacosene (C26:1)	18.131	18835-33-1	500
Not identified, may be alifatic compound and possibly alcohol functionality	18.223	-	2.7
Not identified	18.871	-	4.2
Octacosene (C28:1)	19.649	18835-34-2	350
Not identified	20.34	-	3.8
Triacontene (C30:1)	21.069	18435-53-5	150
Dotriacontene (C32:1)	22.586	18435-55-7	35
Tris(2,4-di-tert-butylphenyl) phosphite	24.193	31570-04-4	220
Tetratriacontene (C34:1)	24.414	61868-12-0	6.7

*: Expressed as mg component as naphthalene equivalent per kg product simulant



GC/MS chromatograms of sample 970130-1 at the top, 970130-2 in the middle and 970130-3 at the bottom. Note that all three chromatograms are similar in being dominated by aliphatic compounds eluting at regular intervals. All samples showed a relatively high concentration of linear aliphatic compounds, where sample 970130-1 contained saturated compounds and sample 970130-2 and 970130-3 contained unsaturated compounds.

Comments

The highest concentrations of PE phenols (degradation products of antioxidants and stabilisers) were observed in the product simulant from sample 970130-1 and 970130-3, and the most dominant components were 7,9-di-tert-butyl-1-oxaspiro(4,5)decra-6,9-diene-2,8-dione (CAS no. 82304-66-3) and 3-methyl-3,5-di-tert-butyl-4-hydroxyphenyl-propanoate (CAS no. 6386-38-5).

PAH compounds were not observed above the detection limit in any of the samples.

The GC/MS screenings showed a large number of compounds with most compounds present in low concentrations. The most dominant compounds were linear aliphatic compounds. In sample 970130-1 the dominant compounds were saturated whereas the dominant compounds were unsaturated in sample 970130-2 and -3. The reason for this is not known. It is noted that the position of the double bound is not well determined by qualitative GC/MS, and that the MS spectrum from an alkene is very close to the MS spectrum for the corresponding primary alcohol of same chain length.

Appendix 3. Excel tool for the screening of identified components in recycled plastic (PCR post-consumer recycled plastic)

Appendix 3.1 Introduction

During the project “Initial safety assessment of recycled plastic for packaging of cosmetic products” from 2020 (ref. /1/), a long list of substances identified in recycled plastic materials to be used as packaging materials for cosmetic products were found by chemical analysis. A human risk assessment of a few of these substances was carried out. However, no further assessment was done for the rest of the substances. Therefore, a hazard screening of these remaining non-assessed substances may give an overview of whether some of these substances are of concern. Therefore, DHI A/S was requested to prepare an excel-based tool, where it is checked if the identified substances in the above mentioned analyses are placed on various lists of substances identified to be of concern.

Appendix 3.2 Substances included

The basic idea is to create a database (in excel) including all identified substances in the recycled plastic materials (also including those included in the risk assessment).

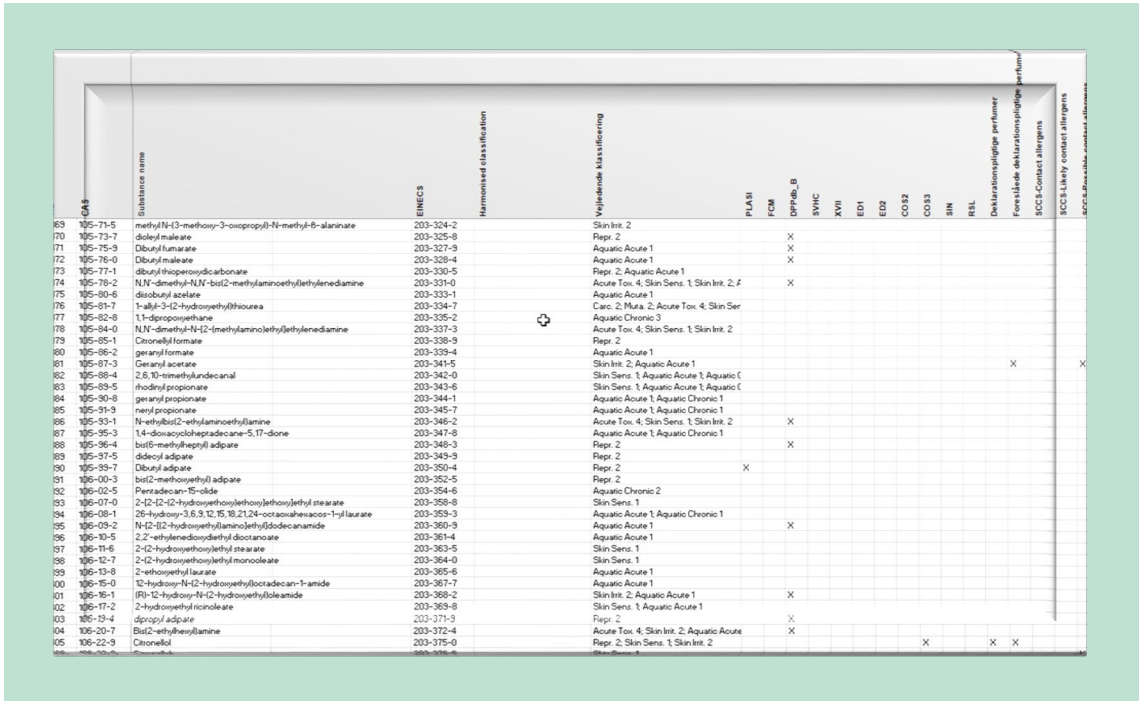
The identified substances will be compared to two types of external public lists:

- Existing lists of chemical substances known to be used in plastic
- Existing lists of chemical substances of concern.

DHI A/S received an excel-fil with the analysis results. These were organised into an overall excel-file. One substance may well be present several times, as different types of chemical analysis have taken place. Distinction is made between these analyses.

In addition, the results of the analysis of the virgin PE (Appendix 2) was included in the excel-file.

The lists are organized in one sheet, with a long list of possible cas-numbers, and then it is marked with a “X” if the substance is on the considered list.



	CAS	Substance name	EINECS	Harmonised classification	Vejledende klassificering	PLASI	FCM	DPPAb_B	SVHC	XVII	ED1	ED2	CO S2	CO S3	SIN	RSL	Deklarationspligtige parfumer	Foreslåede deklarationspligtige parfum	SCCS-Contact allergens	SCCS-Likely contact allergens	SCCS-Possible contact allergens
69	105-71-5	methyl N-(3-methoxy-3-oxopropyl)-N-methyl-ß-alaninate	203-324-2		Skin Irrit. 2																
70	105-73-7	dioleyl maleate	203-325-8		Repr. 2			X													
71	105-75-9	Dibutyl fumarate	203-327-9		Aquatic Acute 1			X													
72	105-76-0	Dibutyl maleate	203-328-4		Aquatic Acute 1			X													
73	105-77-1	dibutyl thioperoxydicarbonate	203-330-5		Repr. 2; Aquatic Acute 1																
74	105-78-2	N,N'-dimethyl-N,N'-bis(2-methylaminoethyl)ethylenediamine	203-331-0		Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2; A			X													
75	105-80-6	diisobutyl azelate	203-333-1		Aquatic Acute 1																
76	105-81-7	1-allyl-3-(2-hydroxyethyl)thiourea	203-334-7		Carc. 2; Muta. 2; Acute Tox. 4; Skin Ser																
77	105-82-8	1,1-dipropoxyethane	203-335-2		Aquatic Chronic 3																
78	105-84-0	N,N'-dimethyl-N-[2-(methylamino)ethyl]ethylenediamine	203-337-3		Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2																
79	105-85-1	Citronellyl formate	203-338-9		Repr. 2																
80	105-86-2	geranyl formate	203-339-4		Aquatic Acute 1																
81	105-87-3	Geranyl acetate	203-341-5		Skin Irrit. 2; Aquatic Acute 1														X		X
82	105-88-4	2,6,10-trimethylundecanal	203-342-0		Skin Sens. 1; Aquatic Acute 1; Aquatic C																
83	105-89-5	rhodinyl propionate	203-343-6		Skin Sens. 1; Aquatic Acute 1; Aquatic C																
84	105-90-8	geranyl propionate	203-344-1		Aquatic Acute 1; Aquatic Chronic 1																
85	105-91-9	neryl propionate	203-345-7		Aquatic Acute 1; Aquatic Chronic 1																
86	105-93-1	N-ethylbis(2-ethylaminoethyl)amine	203-346-2		Acute Tox. 4; Skin Sens. 1; Skin Irrit. 2			X													
87	105-95-3	1,4-dioxacycloheptadecane-5,17-dione	203-347-8		Aquatic Acute 1; Aquatic Chronic 1																
88	105-96-4	bis(6-methylheptyl) adipate	203-348-3		Repr. 2			X													
89	105-97-5	didecyl adipate	203-349-9		Repr. 2																
90	105-99-7	Dibutyl adipate	203-350-4		Repr. 2	X															
91	106-00-3	bis(2-methoxyethyl) adipate	203-352-5		Repr. 2																
92	106-02-5	Pentadecan-15-olide	203-354-6		Aquatic Chronic 2																
93	106-07-0	2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethyl stearate	203-358-8		Skin Sens. 1																
94	106-08-1	26-hydroxy-3,6,9,12,15,18,21,24-octaoxahexacos-1-yl laurate	203-359-3		Aquatic Acute 1; Aquatic Chronic 1																
95	106-09-2	N-[2-[[2-hydroxyethyl]amino]ethyl]dodecanamide	203-360-9		Aquatic Acute 1			X													
96	106-10-5	2,2'-ethylenedioxydiethyl dioctanoate	203-361-4		Aquatic Acute 1																
97	106-11-6	2-(2-hydroxyethoxy)ethyl stearate	203-363-5		Skin Sens. 1																
98	106-12-7	2-(2-hydroxyethoxy)ethyl monooleate	203-364-0		Skin Sens. 1																
99	106-13-8	2-ethoxyethyl laurate	203-365-6		Aquatic Acute 1																
100	106-15-0	12-hydroxy-N-(2-hydroxyethyl)octadecan-1-amide	203-367-7		Aquatic Acute 1																
101	106-16-1	(R)-12-hydroxy-N-(2-hydroxyethyl)oleamide	203-368-2		Skin Irrit. 2; Aquatic Acute 1			X													
102	106-17-2	2-hydroxyethyl ricinoleate	203-369-8		Skin Sens. 1; Aquatic Acute 1																
103	106-19-4	dipropyl adipate	203-371-9		Repr. 2			X													
104	106-20-7	Bis(2-ethylhexyl)amine	203-372-4		Acute Tox. 4; Skin Irrit. 2; Aquatic Acute			X													
105	106-22-9	Citronellol	203-375-0		Repr. 2; Skin Sens. 1; Skin Irrit. 2										X			X	X		

FIGURE 4. Organisation of the public list in the excel-database.

Appendix 3.3 CAS-number check

The CAS-number is used as the key for checking if a substance is on a list or not. However, it is a challenge that the CAS-number is not always unique – meaning for example that a specific substance may actually have more than one CAS-number assigned.
An illustrative example of this inherent difficulty is DEHP. Its main cas-number is 117-81-7 - however DEHP has also been assigned the CAS-number 74746-55-7 in some of the reported analysis in ref./1/. The CAS-number 74746-55-7 is not found in the ECHA database. However, when googling the 74746-55-7, then the PubChem refers correctly to Bis(2-ethylhexyl) phthalate (CID 8343) – even though the PubChem document does not refer to this CAS-number in the substance PubChem Entry. In addition, other CAS-numbers may be assigned to DEHP, namely 82208-43-3, 15495-94-0, 52622-73-8, 8033-53-2. In addition, a number of deprecated CAS-numbers are assigned to DEHP: 126639-29-0, 137718-37-7, 205180-59-2, 40120-69-2, 50885-87-5, 8033-53-2, 275818-89-8, 109630-52-6, 607374-50-5.
Our solution to this challenge was to search the PubChem database for each of the reported CAS-numbers in the chemical analysis, and then to include all assigned CAS-numbers mentioned in the PubChem in the check of if the substance is on one of the involved lists reported in section 2.2. This may not give a 100% guarantee of that all matches are found. In addition, if two cas-numbers are reported for the same substance then a check of if the substance is on one of the involved lists for both cas-numbers are made.

Appendix 3.4 Organisation of the excel-file

The excel-file contains four sheets:
ReadMe: this sheet contains short introduction on how to operate the excel-file.
Summary: This sheet is the key sheet containing all the information i.e., analysis results, max. concentration in the samples, the results of the virgin polymer analysis, indication of if the substance is found on one or more of the lists. Note that some of the columns are hidden; e.g.

- ***Column D***: this column contains the chosen unique name of the substance. It was necessary to include this column, as the naming of the substances in the analysis report was not completely consistent. It should be noted that this column is used for the sorting of the results.
- ***Column F***: additional cas-number as reported in the analysis report
- ***Column G-H***: cas-numbers without hyphen
- ***Column I***: A unique substance ID number has been assigned. This was introduced in order to be able to group different cas-number into one single substance group
- ***Column J-L***: analysis results for the virgin polymer
- ***Column M-S***: analysis results for the PCR

CASNumberCheck (hidden as default): This sheet contains all cas-number assigned to each substance
TotalList (hidden as default): This sheet contains a list of all substances listed on the various lists. See Tabel 1 for information on the structure.

Appendix 3.5 Other elements in the excel-file

During this project, a need for additional data was identified. Therefore, additional information for some of the substances were provided:
Column DH: DHI has added information of relevance for the assessment of the substance
Column DI-DK: DNEL (Derived No Effect Levels) given in the REACH registration dossier for the oral, dermal (general public), dermal (occupational)
Column DL-DN: Absorption values given in the REACH registration dosser (dermal, oral, inhalation respectively)
DO-DP: Calculated dermal absorption using the programme FiniteDoseSkinPerm from respectively a solution of olive oil (column DO) and water (column DP).
DR-EP: EpiSuite calculation results:

- Kp: dermal permeability coefficient
- DA event mg/cm2: dermally absorbed dose per event
- DAD mg/kg/d: Dermal Absorbed Dose (DAD) of organic compounds via water contact.
- Mw: molar mass
- LogKOW: netto logKOW: = measured logKow is available – otherwise calculated logKOw
- Sw (mg/cm3): water solubility (mg/cm3)
- Vp (Pa): vapor pressure
- VP@temp: temperature at which the vapor pressure is given
- SW: water solubility (mg/L)
- SW@temp: temperature at which the water solubility is given
- LogKow: calculated logKow
- logKow, exp: measured logKow

Problematic chemicals in recycled plastic intended for cosmetics packaging
Assessing the safety of post-consumer recycled plastic (PCR) in contact with cosmetic products is difficult, because of the immense numbers of substances which may migrate from the plastic packaging into the cosmetic product. In this report, we provide the technical basis for developing criteria for two lists of hotspot substances, one for leave-on products and one for rinse-off products. We suggest that this can be used as an element in the quality documentation for the supply chain communication.

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