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Initial safety assessment of recycled plastic for packaging of cosmetic products

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Preface

This report describes the results of the project on initial safety assessment of recycled plastic for packaging of cosmetic products such as shampoo, body lotion or liquid soap. The recycled plastic in focus is *post-consumer recycled plastic* (PCR plastic) obtained from relevant stakeholders in the Danish industry. Initially, the PCR material samples with accompanying documentation were collected and assessed, and then specific samples were selected for analysis and safety assessment. An analysis program for migration studies followed by broader screenings of ingredient substances and substance-specific analyses were combined and carried out to generate knowledge on the chemistry in PCR materials. Finally, a safety assessment was performed for specific chemical substances in selected PCR materials based on the results of chemical analysis.

The project was carried out during the period from August to December 2020 for Danish Environmental Protection Agency by Danish Technological Institute with DHI as subcontractor.

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Summary and conclusion

Danish Environmental Protection Agency has requested further knowledge on opportunities and risks regarding the recycling of household *post-consumer recycled plastic* (PCR plastic), for polyethylene (PE) and polypropylene (PP) plastic types in particular. The focus is on recycling of PCR plastic for packaging of cosmetic products as the cosmetic industry requires guidelines to be able to guarantee the safety of the products.

Thus, the aim of this project is to generate knowledge and data on PCR plastics, which can contribute to creation of guidelines for the cosmetics industry on how PCR plastic can be safety assessed in future, and hereby be used safely for packaging of cosmetic products for personal care (e.g., shampoo, body lotion or liquid hand soap).

The focus is on creating an understanding of which chemical substances can potentially constitute a risk of migration from packaging made from PCR plastic into the cosmetic products (in this project, the term “packaging” has been used to denote primary packaging or container that is in direct contact with the cosmetic product). The analyses and assessments of PCR plastic samples in the project will constitute examples, which can later be included as cases for the creation of guidelines for the cosmetics industry. Furthermore, the project has identified a possible need for further scientific knowledge on PCR plastic for the creation of guidelines.

Collected PCR plastic samples
Prior to the project, the Danish Environmental Protection Agency had invited Danish companies to provide samples and documentation for PCR plastics. At the beginning of this project, documentation and sample materials for 17 different PCR plastic fractions in total were received from five suppliers: one plastics processing company and four packaging and cosmetics production companies, who had delivered PCR plastic samples from their own supply chain. The samples were then assessed according to type, documentation, appearance an odor, and prioritized for further analysis.

The received documentation usually contains a description of the type of plastic, waste source, origin, and possible sorting and reprocessing process. 13 samples of HDPE and 4 samples of PP were received. Three main waste sources are represented in the samples: 11 samples originate from household polymer-sorted plastic, 4 samples are based on fishing equipment, and 2 samples come from collected plastic waste from oceans, rivers, and beaches in the Indian Ocean. There are also samples from Denmark, other EU-countries, and countries outside the EU.

For 15 out of 17 samples, the documentation contains technical/physical data for PCR materials, typically in the form of melt flow index (MFI) and density, and sometimes supplemented by mechanical properties. As for the melt flow index for HDPE samples, these indicate that the plastic material is suitable for bottle blowing, while those of PP-samples are slightly higher. For most of the samples, the suppliers have assessed that the material properties of the PCR material make it suitable for packaging material according to normal function requirements to packaging material properties (e.g., flow properties and strength). However, a few suppliers are skeptical as to the odor of the PCR material.

Regarding the chemical content of PCR materials, it has been stated for many of the samples whether a SVHC-content above 0.1% have been detected according to REACH Regulation, and whether the sample complies with RoHS requirements to the content of selected sub-

stances with a threshold value of max. 0.1%. For 5 out of 17 samples, data on overall migration limit (OML) for non-volatile mass from the material have been indicated, which all comply with the general requirements for migration from food packaging (according to Commission Regulation (EU) No 10/2011). However, it is the content and migration of specific substances (especially, organic compounds) that ultimately determines the quality and application possibilities for PCR material, but this information regarding PCR materials is very limited. Documentation for migration of specific substances is only indicated for 2 samples and only for metals.

In general, the received documentation is of usable quality, although it has been necessary to supplement it with additional contact to suppliers to obtain supplementary information. However, the documentation on migration of the specific substances is not adequate to be able to assess whether PCR materials are safe for use in packaging of cosmetic products.

An introductory quality assessment of the received PCR plastic samples was performed as a simple assessment of appearance and odor. The color of most PCR plastic samples is light (that is, whitish, greyish, off-white), while five of the samples are darker (greenish). Odor assessment showed that odor could be detected in all samples.

According to the information in the received documentation and the initial quality assessment, 7 samples in total were selected for screening out of which 4 were selected for a detailed analysis. The samples were selected in cooperation with the Danish Environmental Protection Agency, so that they represent different suppliers/manufacturers as much as possible, both PE and PP plastics, PCR plastics in (expected) high and low quality, as well as PCT plastics from different waste sources and geographic locations.

Assessment and analysis strategy

To be able to carry out a safety assessment of a PCR plastic sample intended for use as packaging material for cosmetic products, it is necessary to know which (concentrations of) chemical substances can migrate from packaging plastic into the cosmetic product. To investigate this, a chemical product simulant was selected, which simulates a specific product type, and a migration study was performed on the plastic material with this product simulant as migration liquid. An important element in this project is thus the developed analysis strategy which includes the selection of product simulant and migration setup as well as the prioritization of chemical substances for analyses. These choices form the basis of the analysis program of this project, so that the safety assessment of PCR materials can be performed based on the results of the performed chemical analyses.

Product simulant and migration conditions

Since the aim of this project is to investigate the migration to cosmetic products, it may be relevant to use both polar and non-polar simulants, which will be representative of water-based and fat-/oil-based cosmetic products. However, it is estimated that the use of a non-polar, fat-dissolving product simulant for migration analysis will be a worst-case scenario with the greatest risk of migration both for most migratory additives from plastic and for those substances that have been migrating into the plastic during the use and lifetime of the plastic (since polyolefins themselves are non-polar). In this project, isooctane and 95% ethanol are used as product simulants, as these can be considered as a realistic worst-case scenario in relation to a fatty product, such as skin cream. Both 95% ethanol and isooctane are used in different migration studies to provide optimal solvent conditions for the relevant analysis apparatus. Thus, isooctane is used for gas chromatography, while 95% ethanol is used for liquid chromatography. Lastly, migration is also performed with 3% acetic acid as product simulant due to the analytical technical conditions for chemical analysis of PAA and migration of metals.

Migrations should take place within the same time as one might expect a product to be contained in a given packaging, but instead of long-term migration tests, accelerated tests were

performed by increasing the temperature, which in turn increased the migration rate of components in PCR material. As a realistic scenario for safety assessment of PCR plastic fractions of HDPE and PP, migration was carried out for three days at 60 °C to simulate a 12-month storage of product simulants in packaging of PE/PP, according to guidelines from the Joint Research Centre (JRC) of the European Commission.

Chemical analyses
After migration from PCR plastic into a product simulant, the content of unwanted chemical substances in the simulant has been examined. Even in virgin plastic, many potentially hazardous substances can be detected, for example, residues of monomers, solvents, impurities, additives, oligomers, and degradation products from the plastic material. Furthermore, in the phases of usage and waste management, a mixing with other materials, which may be absorbed into the plastic, can occur. The greatest challenge is that it is not known what to look for in the analyses, and, furthermore, it is not possible to exclude that there is a significant variance in the material. Since it is not possible to perform analyses on all possible chemical substances in the samples, it was decided in this project to perform three screening analyses supplemented by specific analyses of selected substances/groups of substances.

The content of unknown chemical compounds that may have migrated into the plastic during its usage and lifetime is relevant based on the perspective that the history of plastic is unknown. A large part of these problematic substances can be examined by GC/MS screening, as this method is suitable for identifying a large part of the chemical substances (boiling point below 500 °C), which can migrate across skin barrier.

Furthermore, the samples are screened in LC/MC-multitarget analysis specifically developed for the analysis of unknown substances in plastic materials in connection with food contact material analysis. This method offers a higher sensitivity compared to a GC/MS screening.

Finally, ICP/MS screening is included in the analysis program to examine the migration of 64 different metals, including chromium, cobalt, nickel, and aluminum, which are interesting due to their allergenic effects, and heavy metals, such as cadmium, mercury, arsenic, and lead, which are unwanted in products due to their health-related effects.

In addition to screenings, specific analyses were performed for selected substances/groups of substances, which are considered relevant in relation to the following safety assessment of PCR plastic material. Also, it must be emphasized that the selected substances do not constitute an exhaustive list of substances relevant to analyze in connection with a safety assessment of PCR plastic materials. The substances are prioritized in the project based on the experiences and knowledge of the project group on PCR plastic, problematic substances, and available analysis methods. The following substances have been selected for substance-specific analyses:

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

- Total fluoride content, which is measured to obtain an indication of whether other per-fluoroalkyl and polyfluoroalkyl substances, other than the selected PFAS, can be included, which are analyzed with the above-mentioned PFAS measurement.

According to the above-mentioned description, the analysis program of this project can be summarized as shown in TABLE 1.

TABLE 1 Overview of project analysis program.

Analyzed substances	Analysis method	Product simulant (migration 3 days, 60 °C)	Number of samples
(Screening)	GC/MS	Isooctane	7
(Multitarget-analyses)	LC/MS	95 % ethanol	7
(Screening of) selected metals	ICP/MS	3 % acetic acid	4
PAH	GC/MS	Isooctane	4
PAA	LC/MS/MS	3 % acetic acid	4
PE-phenols (breakdown products from antioxidants and stabilizers)	GC/MS	95 % ethanol	7
Perfluoroalkyl and polyfluoroalkyl substances (PFAS)	LC/MS/MS	(Content analysis)	4
Total content, fluorine	EN 14582:2016	(Content analysis)	4

Migration studies and chemical analyses

Migration studies primarily show that some samples discolor the product simulant. This means that PCR plastic packaging can potentially discolor the packaged cosmetic products, and thus change the visual appearance of, for example, a cream, which can be problematic.

Screening analyses

The total amount of analyzable organic substances varies from 980 mg/kg to 7700 mg/kg. The GC/MS screenings detect a high number of non-aromatic aliphatic compounds, where the majority are found to be saturated. The content of non-aromatic unsaturated aliphatic compounds is the largest group of chemical components detected. These are linear and branched aliphatic compounds, and since they are found in all samples, it may indicate a degradation of the primary (polyolefin-)polymer chain. In addition, PCR plastic samples show a great difference in the number of components and the amount of non-aliphatic components. This group includes, for example, additives, degradation products from additives and substances, which can be absorbed or adsorbed during the lifetime of plastic, e.g., at the consumer.

The GC/MS screenings detected various esters and terpenes, which may influence the olfactory properties and the relatively high amounts of degradation products from antioxidants and stabilizers. In several samples, the content of legally (REACH) restricted phthalates, such as DBP, DIBP, BBP DEHP was detected. The content is relatively low (below 0.005 % in all cases), but it may influence the product's access to the market.

LC/MS multitarget analysis detected a range of different components related to the production and processing of plastic, including softening agents and polymerization agents. Softening agents are not added to virgin polyolefins but may occur as contaminants during processing. Most of the detected components are present at a level of approx.1 mg/kg in the applied product simulant.

ICP/MS screening detected a small number of metals, which have migrated into the product simulant. No content has been found of the metals typically associated with allergies, i.e.,

nickel, chromium, and cobalt. However, the content of approx. 0.5 mg/kg aluminum was found in the product simulant in several samples. During screening, the content of problematic heavy metals, such as cadmium, mercury, arsenic, or lead was not detected above the specified detection limit.

Substance-specific analyses
Several PAH-compounds were found in the product simulant in an amount, which makes it not possible to disregard. REACH restricts PAH in toys and 'childcare articles', which come into long-term contact with the throat or skin, to 0.5 mg/kg for eight chosen compounds, and if the content exceeds 1 mg/kg, the product cannot be marketed.

The analyses for PAA indicated the presence of both 4,4'-diaminodiphenylmethane and o-Toluidine in small amounts in all four analyzed samples, while one of the samples contained additional four PAAs.

No content or traces of fluorene substances was found either by component-specific analysis or analysis for total fluoride content.

Safety assessment
Based on analysis results and due to the limitations of this project, a small selection of the identified substances has been prioritized for specific safety assessment based on the following substance properties:

- Allergens, CMR-substances, or substances considered to be endocrine disrupting.
- Substances in Annex II of Regulation (EC) No 1223/2009 on cosmetic products.
- Substances, which appear to migrate from several analyzed samples, and/or in concentrations higher than allowed in plastic approved as food contact materials (FCMs).

The following substances/groups of substances have been selected for safety assessment:

- Aluminum due to allergenic effects.
- Phthalates: dibutyl phthalate (DBP), benzyl butyl phthalate (BBP) and bis(2-ethylhexyl) phthalate (DEHP) due to frequent occurrence in the samples and classification.
- Benzophenone due to high concentration, frequent occurrence in samples as well as very low tolerable daily intake (TDI).
- Tris-(2,4-di-t-butylphenyl)phosphite due to frequent occurrence and high concentration in samples.
- 2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT) due to frequent occurrence and high concentration in samples. BHT is allowed as antioxidant in cosmetics, but it currently under assessment as endocrine disrupting.
- 2,4-Di-tert-butylphenol – as it is a frequently occurring degradation product of antioxidants in plastic, and since it has a low threshold value in drinking water.

Safety assessment has been carried out according to the results of the performed analyses based on the existing guidelines for the assessment of ingredient substances in cosmetic products by SCCS. An exposure scenario has been created for baby body lotion (as a representative for worst-case exposure of a leave-on product), and for shampoo for adults (rinse-off) with short-term exposure, as a contrast).

Based on the analysis results for the above-mentioned substances in seven analyzed PCR-plastic samples, the maximum acceptable concentrations for substances were calculated for two exposure scenarios (baby body lotion and shampoo). The calculated concentrations have been compared to the analyses results in TABLE 2, where the measured concentrations above the maximum acceptable concentrations are shown in red.

It can be seen that the concentration of 2,4-di-tert-butylphenol exceeds the acceptable concentration in baby body lotion for six out of seven samples, and two of the samples further exceed the acceptable concentration in baby body lotion for other compounds (tris-(2,4-di-t-butylphenyl)phosphite and the phthalates DEHP and DBP). Thus, based on the assumptions and methods in this project, it is assessed, except for sample no. 1.1, that PCR materials cannot be used directly as packaging for baby body lotion. In case of shampoo, it is possible to see in the table below that there are no exceeded limits of the calculated acceptable concentration for the selected substances. Thus, it cannot be ruled out that the seven PCR materials can be used as packaging for shampoo if the remaining detected substances are otherwise considered safe for use.

In the risk assessment of exposure scenarios, the margins of safety (MOS) were also calculated by taking the different absorption properties into account. In the assessment of MOS values and whether risks are present, uncertainty factors, exposure estimates (including exposure from other sources), and experimental data that form the basis for NOAEL/LOAEL value are included. Since a TDI or DNEL value is available for the selected substances, the MOS value of 10 can be accepted, as 10% of TDI is allocated to cosmetic products. This allocation allows additional exposure from other sources such as drinking water and food.

TABLE 2 Comparison of analysis results and the calculated maximum acceptable concentrations in baby body lotion and shampoo, respectively. Numbers in red indicate that the maximum acceptable concentration in baby body lotion is exceeded. No measured concentrations exceed the maximum acceptable concentration in shampoo.

Name of substance	CAS No.	Max. acceptable conc. (mg/kg) Baby body lotion Shampoo	Measured conc. (mg/kg) Sample 1.1	Measured conc. (mg/kg) Sample 2.1	Measured conc. (mg/kg) Sample 3.3	Measured conc. (mg/kg) Sample 3.5	Measured conc. (mg/kg) Sample 4.2	Measured conc. (mg/kg) Sample 5.3	Measured conc. (mg/kg) Sample 5.4
Benzophenone	119-61-9	**13** **9799 (0.9%)**	1.2	0.59	2.2	0.25	-	-	0.58
Dibutyl phthalate (DBP)	84-74-2	**20** **1315 (0.1%)**	0.098	0.14	7.8	0.54	0.24	4.5	1.8
Diethylhexyl phthalate (DEHP)	117-81-7	**295** **19595**	5.6	-	42	220	44	10	-
Sum of DEHP, DBP (x5)	-	**148** **9798**	6.1	-	81	**223**	45	33	-
Tris(2,4-di-t-butylphenyl)phosphite	31570-04-4	**190** **11757**	110	140	-	22	**1000**	-	3.8
2,4-Di-tert-butylphenol	96-76-4	**2** **150**	-	**2.2**	**4.1**	**2.0**	**4.5**	**6.5**	**4.6**
2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	**550** **36560**	0.33	0.38	1.7	0.67	-	5.9	2.4
Other substances (triviality limit)	-	**0.0008** **0.049**							

Conclusions

Generally, the safety assessment of the selected substances/groups of substances in the examined PCR plastic materials show that plastic materials could be used as packaging for certain cosmetic products. The usage of PCR plastic in packaging for shampoo is generally safer compared to baby body lotion, as shampoo is rinsed out after use, and the exposure is typically to a relatively large body weight compared to skin surface.

Seven different PCR plastic samples were analyzed, which does not provide enough information to be able to say anything general about the content of chemical substances in PCR plastic. Samples have been analyzed from different suppliers, plastic waste types and geographic origin, but the data foundation is too small to be able to draw general tendencies regarding the different sources for PCR plastic.

Migration is possible for an infinite number of substances from PCR plastic, as plastic materials can naturally occur from many sources and may have many different applications during their lifetime while being used by the consumer. The analyses have detected many more substances than it was possible to safety assess in this project due to limited resources, and thus the presence of other problematic substances with lower concentrations than the indicated detection limit cannot be ruled out. It is concluded that the relevant analyses carried out within this project provide a broad insight into the chemistry of PCR plastic materials, and that, based on the performed analyses, some problematic components have been selected for a more detailed toxicological investigation to provide examples on safety assessment of PCR plastic for packaging of cosmetic products. A complete safety assessment of a specific PCR plastic material must include all problematic substances that have been detected in chemical analyses and assess these in relation to whether the measured concentrations are safe for the specified usage of the packaging. Furthermore, a complete safety assessment must also assess whether the applied analysis methods can detect all relevant substances in the relevant concentrations. For example, it can be substances, which only migrate by using more polar simulants, and it can also be substances, which due to interference in the analysis cannot be detected or quantified.

In connection with this safety assessment, a general “triviality limit” has been calculated for migration of 0.8 µg/kg product for substances in packaging used for cosmetic products with skin contact. However, if the PCR plastic material is to be used for packaging of hair shampoo, the triviality limit can be increased to 49 µg/kg shampoo. The triviality limit has been calculated based on the equivalence to the most hazardous chemical substances, even though it is highly unlikely that precisely these can be found in PCR plastic. Yet, the calculated triviality limits are so low that they are below the normal detection limits in the analyses that can be performed. Thus, their practical application is limited.

Out of all the substances calculated for in this project, it appears that in many cases 2,4-di-tert-butylphenol exceeds the acceptable level. The component is a degradation product from many different antioxidants which are typically used in PE plastic. In the same way, both phthalates and tris-(2,4-di-t-butylphenyl)phosphite in some cases exceed the acceptable level for baby body lotion.

All PCR plastic samples gave off odor, and fragrance substances were detected in the chemical analyses. This may be a challenge when recycling plastic for packaging, as fragrance substances can migrate from the packaging into the cosmetic product. Furthermore, discolorations are observed in migration studies, which may cause implications for the visual appearance of the visual product when using PCR plastic packaging.

1. Introduction

1.1 Background

According to EU Plastics Strategy, more plastic packaging must be recycled, and Danish authorities, industries and consumers are demanding further recycling of plastic packaging. Initiatives have been started from many parties to clarify how recycled plastic can be used in cosmetic packaging, so that the safety of the product meets the current legislative requirements, and at the same time taking the sustainability of the product into consideration in the best possible way. The same applies also to a larger circular perspective, e.g., by avoiding "downcycling" of high-quality materials.

The industry and authorities pay a special interest to the recycling of household collected post-consumer recycled plastic (PCR plastic), which is the reason why guidelines are requested for such recycling. Already today, recycled PET (recycled polyethylene terephthalate, rPET) is used in the production of e.g. packaging, because PET is available in relatively few different qualities and process-wise is suitable for recycling multiple times. In its virgin form, PET is also widely used in food packaging, providing a greater assurance of quality and purity, as the source would thus often be PET, which is approved for food contact.

It is desired to expand the range of usable processed plastic to achieve a greater degree of recycling. A widely used group of plastic is polyolefins, and hence it would be obvious to recycle these to a greater extent. An increased recycling of polyolefins such as polyethylene (PE) and polypropylene (PP) is more challenging than recycling of PET, as polyolefins occur in many qualities, they are more easily degradable and are used for many different products, including fragranced cleaning agents. Furthermore, they contain several different additives and can thus be contaminated with different substances to a much greater extent than rPET, which makes processing of polyolefins more challenging. Finally, the source of the processed plastic is utmost important for how the plastic can be contaminated. Thus, further knowledge is required in order to overcome these barriers which prohibit a safe recycling of, e.g., packaging products.

Based on the high demand for PCR plastics for recycling in packaging, this project will investigate the presence and migration of chemical substances in several PCR plastic samples. Thereafter, the safety of their application as packaging for cosmetic products for personal care (e.g., shampoo, body lotion or liquid hand soap) will be assessed, as currently, recycled plastic which is approved for food contact is used for this type of products. EU Cosmetics Regulation (EC) No 1223/2009[1] stipulates that a safety report must be created for each cosmetic product, which, among others, includes a safety assessment, where both the packaging and packaging together with the products must be safety assessed. In this project, "packaging" is used to refer to the primary packaging or container that is in direct contact with the cosmetic product.

1.2 Aim

The project must generate knowledge and data on PCR plastic, which can contribute to a later creation of guidelines for the cosmetics industry on how recycled, household-collected plastic (PCR) can be safety assessed and thus can be safely used for packaging of cosmetic products for personal care (e.g., shampoo, body lotion or liquid hand soap).

[1] Regulation (EC) No 1223/2009 of the European Parliament and of the Council of 30 November 2009 on cosmetic products (hereinafter referred to as 'EU cosmetics regulation')

The focus will be on creating understanding of which chemical substance can potentially constitute a risk by migrating from PCR plastic packaging into cosmetic products for personal care. The analyses of PCR plastic samples in the project will create examples, which can later be included as cases for further development of guidelines for the cosmetics industry. The need for further scientific knowledge on PCR plastic needed for the development of guidelines will also be identified in this project.

1.3 List of abbreviations

ADI	Acceptable daily intake (used for substances added intentionally, e.g. food additives and pesticides)
BBP	Butyl-benzyl-phthalate
BHT	2,6-Bis(1,1-dimethyl)-4-methylphenol
Carc.	Carcinogenic
CAS	Chemical Abstract Service
CMR	Carcinogenic, Mutagenic and Reprotoxic. CMR-substances are carcinogenic, mutagenic and reprotoxic substances.
DBP	Dibutyl phthalate
DEHP	Bis(2-ethylhexyl)phthalate
DNEL	Derived No Effect Level, i.e., the highest amount of a chemical substance which a person can tolerate as systemic dose (corresponds mainly to TDI).
ED	Endocrine Disruptor
ECHA	European Chemicals Agency
EFSA	European Food Safety Authority
FCM	Food contact material
GC/MS	Gas chromatography/mass spectrometry
GC-FID	Gas chromatography flame-ionization detection
HAC	Acetic acid
HDPE	High-density polyethylene
ICP/MS	Inductively coupled plasma mass spectrometry
LC/MS	Liquid chromatography/mass spectrometry
LC/MS/MS	Liquid chromatography/mass spectrometry/mass spectrometry
LOAEL	Lowest Observed Adverse Effect Level, i.e., the lowest test dose with effects still visible (used, where NOAEL cannot be detected)
MFI	Melt Flow Index
MOAH	Mineral oil aliphatic hydrocarbons
MoS	Margin of Safety
MOSH	Mineral oil saturated hydrocarbons
MS	Mass spectrometry
NIST	National Institute of Standards and Technology
NOAEL	No Observed Adverse Effect Level, i.e., the dose which does not cause hazardous effects
OML	Overall migration limit, overall migration of non-volatile mass
PAA	Primary aromatic amines
PAH	Polycyclic aromatic hydrocarbons
PC	Post-consumer
PCR	Post-consumer recycled
PE	Polyethylene
PET	Polyethylene terephthalate
PFAS	Perfluoroalkyl and polyfluoroalkyl substances
PP	Polypropylene
PVC	Polyvinyl chloride

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.
Repr.	Reproductive toxicity
RoHS	*Restriction of Hazardous Substances*, Directive 2002/95/EC of the European Parliament and of the Council of 27 January 2003 on the restriction of the use of certain hazardous substances in electrical and electronic equipment**.**
rPET	Recycled polyethylene terephthalate, recycled PET
RSD	Relative standard deviation
RT	Retention time, i.e., the time it takes for a component to pass through the column (in mass spectroscopy)
SCCS	Scientific Committee on Consumer Safety - EU's scientific committee for consumer health and safety
SED	Systemic Exposure Dose, the systemic exposure dose, i.e., the dose absorbed in the body.
SML/SMG	Specific Migration Limit. Used in Commission Regulation (EU) No 10/2011 of 14 January 2011 on plastic materials and articles intended for food contact.
SVHC	Substances 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 can cause a toxicological effect. TTC may be used as the tolerable daily intake of substances with missing toxicological data.

2. Collection and assessment of PCR plastic samples

In this chapter, the collection of PCR plastic samples and associated documentation of these from relevant operators of the Danish industry will be described. Thereafter, the initial assessment of PCR plastic materials will be described based on the received documentation and quality assessment according to appearance and odor of samples. Finally, the selection of specific PCR plastic samples for further analysis and safety assessment is described.

2.1 Collection of PCR plastic samples from relevant suppliers

Prior to the project, the Danish Environmental Protection Agency had invited Danish companies to provide samples of PCR plastic and documentation for samples. At the beginning of this project, documentation, and sample materials for 17 different PCR plastic fractions were received from five suppliers: one plastics processing company and four packaging and cosmetics production companies, who had delivered PCR plastic sample from their own supply chain. The samples were then assessed according to type, documentation, appearance an odor and was prioritized as described in the next chapter.

2.2 Assessment of received documentation

Documentation was received for 17 different PCR plastic fractions. An overview of data on material type, waste source (PC, *post-consumer*), sorting process and reprocessing are shown in TABLE 3.

13 samples of high-density polyethylene (HDPE) and 4 samples of PP were received. Three main, varying waste sources are represented in the samples: 11 samples originate from household polymer-sorted plastic, 4 samples are based on fishing equipment, and 2 samples originate from collected plastic waste from oceans, rivers, and beaches in the Indian Ocean. There are also samples from Denmark, other EU-countries, and countries outside the EU.

In Europe, plastics collected from households are typically processed by passing through a Material Recovery Facility (MRF), where plastics are sorted according to polymer type with Near Infra-red scanners (NIR), also supplemented by manual fine sorting. After sorting into polymer types, the plastic is reprocessed, where it is usually divided into flakes, washed, and dried. Hereafter, the plastic flakes are remelted and pelleted into pellets (granules) by an extruder. In connection with, or after extrusion, the plastic can be processed through a thermic odor removal process.

Data on content, migration, and Melt Flow Index (MFI) are shown in TABLE 3. These data are indicated for the granule product without necessarily being related to the potential use as cosmetic packaging material. In general, for many samples it has been stated whether SVHC-substances above 0.1% have been found, according to REACH Regulation (updated in June 2020)[2], and whether the sample complies with RoHS requirements on the content of selected substances with a threshold value of max. 0.1% [3].

[2] 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 (hereinafter 'REACH').

[3] Directive 2002/95/EC of the European Parliament and of the Council of 27 January 2003 on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS, Restriction of Hazardous Substances Directive).

Total migration (OML, overall migration limit) describes the total migration of a non-volatile mass from the material. For 5 of the samples, the analysis values for OML have been indicated, and these comply with the general requirements for migration from food packaging[4], where the threshold value is 10 mg/dm^2. However, the data for content and migration of specific substances determine the quality and the possible applications of the PCR material. The total migration measured directly on granules is not necessarily relevant in this context, as the OML-value is directly dependent on the surface area. Thus, some manufacturers have chosen to give the OML-value for a pre-molded item, where the result to a greater extent can be related to the actual use of the material. It must be noted that the conditions regarding the casting process are not standardized, which gives an unknown variance in the measured migration values.

The information on migration of specific substances from samples is limited. Migration data has been received only on two samples for which only migration analyses on metals (according to toy safety standard EN 71-3 for samples 4.1 and 4.2) and maximal migration of unknown substances are available. Hence, the information is only related to the migration of metals and organic tin, but no data is available for the release of organic substances during migration.

The technical data for PCR plastic samples has not been fully included in the table below, but physical data, such as Melt Flow Index (MFI) and density, also supplemented with mechanical properties (e.g., tensile strength, breaking strength), and material color, are typically included. Such technical data have been indicated for 15 out of 17 PCR plastic samples. Regarding the melt flow index of HDPE samples, the index for all samples with data is in the size interval 0.2-0.8 g/10 min. at 2.16 kg 190 ˚C,[5] which indicates that the plastic material is suitable for bottle blowing. This is in line with the expectation that the typical source of PCR plastic of HDPE is packaging produced by bottle blowing. The data for PP samples has been given for 3 out of 4 products in the interval from 3 to 40 g/10 min. at 2.16 kg 230 ˚C. A part of PP-type PCR plastic is expected to originate from injection-molded containers made of fluid plastic (typically MFI in the size interval 5-25 g/10 min. at 2.16 kg 230 ˚C). If PCR plastic in PP is too thick for the desired use, the plastic can be modified with additives (e.g., peroxides) or by mixing it with a more fluid PP.

Lastly, the suppliers of the different PCR plastic samples were asked “Do you consider that the functionality of the PCR material makes it suitable as a packaging material (based on normal functional requirements for properties and packaging material such as flow properties, strength, barriers and odor)?” The question was answered with “yes”, “no” or “not examined” as indicated in the far-right column of TABLE 3.
It should be noted that for samples no. 1.1 and no. 5.1 it has been indicated that the product is approved as 40 % additive for packaging for chilled milk or cosmetics. However, the origin of this approval has not been indicated.

In general, the received documentation is of usable quality, although it has been necessary to supplement it with additional contact to suppliers to obtain some of the information in TABLE 3. As mentioned, the data for specific migration, which is important for the assessment of the quality of PCR plastic, is very sparse. In a few cases, this data is available for metals, but documentation on the migration of specific organic substances has not been received.

[4] Commission Regulation (EU) No 10/2011 of 14 January 2011 on plastic materials and articles intended food contact, Article 12. (hereinafter 'FCM Regulation)

[5] For sample 3.5, Danish Technological Institute based on additional documentation has estimated that MFI is in the specified interval.

TABLE 3 Data for PCR plastic samples as stated in received documentation.

Sample No	Material type	Waste source	Sorting	Processing	Declared chemical content	Total migration (OML)	Specific migration	MFI (HDPE: 190 °C, PP: 230 °C)	Suitable for packaging[6]
1.1	HDPE PCR	PC	Sorted	Hot-washed, density separated and purified	SVHC <0.1 %, cf. REACH. <0.3 ppm of unknown substances with GC-FID headspace-analysis	Not stated	Not stated	0.6 (2,16 kg)	Yes
2.1	HDPE 50 % PCR	PC bottles, tubs, trays (UK)	MRF with NIR-sorting, metal removal	Division, wash, flotation and density separation, airstream separation, flake sorting, sifting and extrusion. Odor removal process.	SVHC <0.1 %, cf. REACH PAH <0.15 mg/kg	10 % ETOH: 0.1 mg/dm^2 3 % HAC: 0 mg/dm^2 Olive oil: 1.1 mg/dm^2	Not stated	0.2 (2.16 kg)	No (due to odor)
3.1	HDPE >95 % PCR	PC primarily from food packaging (UK)	MRF with NIR-sorting, manual post-sorting	Wash with additives, melt filtration	Not stated	Not stated	Not stated	0.6 (2.16 kg)	Yes
3.2	HDPE >95 % PCR	Unknown source (Europe)	MRF with NIR-sorting	Wash (EUCERTPLAST certified)	Not stated	(Measured on 750 ml bottle) 10 % ETOH, 3 % HAC Olive oil: all <2 mg/dm^2		0.4 (2.16 kg)	Yes
3.3	HDPE >99 % PCR	PC (Haiti, Philippines, Indonesia, Egypt, Brazil)	Manual sorting (also with NIR)	2-step wet division, density separation, hot wash (90 °C + base), drying, dust separation	Not stated	Not stated	Not stated	0.25 (2.16 kg)	Yes
3.4	PP PCR	Hand-sorted food product plastic (India)	Manual sorting and label removal	Hot wash	Not stated	Not stated	Not stated	Not stated	Yes
3.5	HDPE PCR	Household-collected PC (Denmark)	Manual/NIR-sorting	Friction wash, etc.	Not stated	(Measured on 750 ml bottle) 10 % ETOH, 3 % HAC: <1 mg/dm^2 Olive oil: <2 mg/dm^2	Not stated	1.4 (5 kg)	Yes

[6] Sample suppliers' reply to the question: "Do you consider that the functionality of the PCR material makes it suitable as a packaging material (based on normal requirements for properties and packaging material such as flow properties, strength, barriers and odor)?"

Sample No	Material type	Waste source	Sorting	Processing	Declared chemical content	Total migration (OML)	Specific migration	MFI (HDPE: 190 ˚C, PP: 230 ˚C)	Suitable for packaging[6]
3.6	HDPE PCR	PC bottles (India)	Manual sorting after plastic triangle	Not stated	Not stated	Not stated	Not stated	Not stated	Yes
4.1	HDPE Ocean	Primarily fishnet (Europe)	Manual	Special reprocessing technology	SVHC <0.1 %, cf. REACH. RoHS OK	Not stated	EN71-3: Metals	0.6 (2.16 kg)	Yes
4.2	PP Copolymer Ocean	Primarily cord/net of PP Copolymer (Europe)	Manual	Special reprocessing technology	SVHC <0.1 %, cf. REACH. RoHS OK, phthalates, PAHs, metals, brominated flame retardants	Not stated	EN71-3: Metals	Approx. 3 (2.16 kg)	Yes
4.3	HDPE	Net, flower industry (Europe)	Manual	Special reprocessing technology	SVHC <0.1 %, cf. REACH.	Not stated	Not stated	Approx. 0.8 (2.16 kg)	Yes
4.4	HDPE Ocean	Primarily fishnet (Europe)	Manual	Special reprocessing technology	SVHC <0.1 %, cf. REACH.	Not stated	Not stated	Not stated	Yes
5.1	HDPE PCR	PC	Sorted	Hot-washed and purified	SVHC <0.1 %, cf. REACH. <0.3 ppm of unknown substances with GC-FID headspace-analysis	Not stated	GC-FID < 10 ppb	0.6 (2.16 kg)	Yes
5.2	HDPE 50 % PCR	Not stated	Not stated	Not stated	Not stated	10 % ETOH: 0.6 mg/dm^2 3 % HAC: 4.8 mg/dm^2 Olive oil: 5 mg/dm^2	Not stated	0.6 (2.16 kg)	No (due to odor)
5.3	PP Ocean PCR	PC plastic from oceans, rivers, beaches (Indian Ocean)	Collected plastic is sorted (possibly manually)	Wash, addition of additives and pelletization	SVHC <0.1 %, cf. REACH	10 % ETOH: <1 mg/dm^2 95 % ETOH: 2,8 mg/dm^2 3 % HAC: <1 mg/dm^2 Isooctane: 3,6 mg/dm^2	Not stated	40 (2.16 kg)	Not examined
5.4	PE Ocean PCR	PC plastic from oceans, rivers, beaches (Indian Ocean))	Collected plastic is sorted (possibly manually)	Wash, addition of additives and pelletization	SVHC <0.1 %, cf. REACH	Not stated	Not stated	0.9 (2.16 kg)	Yes
5.5	PP 95 % PCR	PC plastic (Europe)	Collected PC sorted	Not stated	<0.2 % volatile substances, 120 ˚C	Not stated	Not stated	16 (2.16 kg)	Not examined

2.3 Initial assessment of PCR plastic fractions

Picture documentation of received samples is shown in Appendix 1. An initial quality assessment of the received PCR plastics has been performed in the form of a simple judgement of sample appearance and odor. This assessment is summed up in TABLE 4, where the odor has been assessed on a scale from 1 to 5, where 5 represents the strongest odor. The odor assessment was carried out individually by three specialists associated with the project. Thus, it is not an independent panel, which is why it is only an indicative assessment. However, it must be noted that the panel agreed on the following observations:

- Odor was detected in all samples; most of them had an odor of fragrance, fabric softener, soap or similar.
- Sample No. 2.1 and 5.4 emitted the least odor.

TABLE 4 Assessment of PCR plastic samples.

		Odor average		
Sample No.	**Color**	**Scale 1-5**	**Standard deviation**	**Odor description**
1.1	Natural	2.0	0.0	Fragrance, fabric softener
2.1	White/natural	1.0	0.0	Very weak fragrance/odor
3.1	Grey	2.0	1.0	Fragrance, slightly burnt
3.2	White	3.0	0.0	Fragrance, burnt, masking agent
3.3	Natural	3.0	0.0	Burnt, oil/solvent, sulfur compound
3.4	White	1.7	0.6	Plastic-like, acidy smell
3.5	Grey	1.3	0.6	Plastic-like, slightly burnt
3.6	Dark grey	2.7	0.6	Fragrance, musk
4.1	Black	2,3	0,6	Fish-like, indescribable, ‘old’, burnt, unpleasant
4.2	Dark green	3.7	1.2	Fish-like, synthetic, burnt, unpleasant
4.3	White/natural	3.0	1,0	Fish-like, coal, burnt, tar
4.4	Light green	2.3	0.6	‘Chemical’, indescribable, ‘old’, burnt
5.1	Natural	2.3	1.2	Fragrance, fabric softener, soap
5.2	Natural	3.3	1.2	Fragrance, fabric softener, soap, another odor
5.3	White	2.0	0.0	Melted plastic, indescribable, slightly irritating, burnt, ‘old’
5.4	White	1.0	0.0	Plastic-like, no odor (packaging)
5.5	White	1.5	0.0	Fragrance

2.4 Selection of samples for analysis

Based on the information in the received documentation and the initial quality assessment, 7 samples have been selected for screening, and 4 out of these samples have been selected for a detailed analysis. The selected samples are marked in TABLE 5 below. The samples have been selected in collaboration with the Danish Environmental Protection Agency, so that they as far as possible represent:

- Different suppliers and manufacturers
- PCR plastic of both PE and PP
- PCR plastic, which is expected to be documented to a high quality
- PCR plastic, which is expected to be of lower quality (only one sample)
- PCR plastic of different geographic origins
- PCR plastic based on household-collected plastic and plastic from marine environment (i.e., fishing equipment or plastic waste collected from oceans, rivers, or beaches).

TABLE 5 Selection of PCR plastic fractions for analysis.

Sample No.	Material type	Selected for screening	Selected for detailed analysis	Reason for selection
1.1	HDPE PCR	X	X	The only sample from this supplier. Expected of high quality due to appearance and documentation.
2.1	HDPE 50 % PCR	X	X	The only sample from this supplier. Expected of high quality due to waste source (UK), documentation and very weak odor.
3.1	HDPE >95 % PCR			
3.2	HDPE >95 % PCR			
3.3	HDPE >99 % PCR	X		Expected low quality due to waste source (PC from Haiti, Philippines, Indonesia, Egypt, Brazil) and strong odor
3.4	PP PCR			
3.5	HDPE PCR	X	X	The only sample based on Danish household-collected plastic.
3.6	HDPE PCR			
4.1	HDPE Ocean			
4.2	PPC Ocean	X		Represents PP plastic and plastic recycled from fishing equipment (Europe).
4.3	HDPE			
4.4	HDPE Ocean			
5.1	HDPE PCR			
5.2	HDPE 50 % PCR			
5.3	PP Ocean PCR	X		PP plastic and plastic collected from marine environment (Indian Ocean).
5.4	PE Ocean PCR	X	X	Plastic collected from marine environment (Indian Ocean) with expected high quality due to a very weak odor.
5.5	PP 95 % PCR			

3. Assessment and analysis strategy

This chapter describes the assessment and analysis strategy of this project in the form of product simulant and migration setup as well as prioritization of chemical substances to be analyzed. These choices create the foundation for the project's analysis program, so that the safety assessment of PCR materials can be performed based on the results of performed chemical analysis.

3.1 Selection of product simulant

Ideally, a migration would be made to a selected product, after which this product would be analyzed. This would provide a realistic migration to a given product however this would require many analyses as each individual product should then be analyzed. It is also complicated to perform the analysis of the product itself because components in products may interfere with what one wishes to analyze for. Thus, a chemically pure product simulant has been chosen, which simulates a given product type. It is desired to investigate the migration to cosmetic products, which is why it is relevant to apply both polar and non-polar simulants.

A polar simulant will be representative of water-based cosmetic products. Chemical substances, which are expected to migrate into polar simulants are, e.g., metals, of which nickel, chromium and cobalt are interesting as these constitute a risk of causing an allergic reaction upon skin contact. However, these will typically be present because of migration from packaging, but also because they are present in the product itself. The relevant plastic matrix in the form of either PP or PE is highly non-polar, and metal species would be locked in polymer structure and would have difficulty moving in the matrix.

A non-polar simulant would be representative of oil-based cosmetic products such as skin cream but are also relevant for water-based cosmetic products with a high tensile surfactant content such as shampoo or other soap-based product types. Chemical substances, which are expected to migrate into this type of simulant, would be additives added before/during the use and lifetime of the plastic product. Since polyolefins have a non-polar matrix, the non-polar substances will be able to migrate into plastic and subsequently migrate out of it again if the plastic is recycled to produce new packaging. In general, this is the case for all products with a content of fat-soluble substances, e.g., HDPE used for containers for cleaner's naphtha. Also, organic substances with a certain polarity will probably, depending on the specific substance in question, be able to migrate when using non-polar simulants.

Thus, it is considered that the use of a non-polar fat-soluble product simulant in migration analyses of the selected PCR plastic samples will cause a worst-case situation with the greatest possible risk of migration both for the largest part of migratory additives from the plastic and for those substances that have been able to migrate into plastic during its use and lifetime.

In general, the selection of product simulants for PCR plastic sample migration analyses can be beneficially developed further on product simulants already used for analyses in similar fields of study. This would increase the opportunity for direct comparison and would also make it easier for the industry to find a commercial laboratory to carry out their own analyses, as there would be a higher probability that the methods would already be implemented. Here, the migration analyses carried out on plastic used for food packaging should be emphasized,

which are regulated by the Commission Regulation (EU) No 10/2011, where vegetable oil, 95 % or isooctane must be used for migration for packaging with direct contact to fat.

In this project, isooctane (CAS No. 540-84-1) and/or 95 % ethanol have been used as non-polar product simulants, as these can be considered as a realistic worst-case scenario in connection with a fat-containing product such as skin cream. Both additives added to plastic during virgin production and substances that could have migrated into plastic while in use by the consumer, could be studied using these product simulants. Whether isooctane or 95 % ethanol is used for the individual analysis is determined by which migration liquid provides optimal solvent conditions for the relevant analysis equipment. This way, isooctane is used for gas chromatography, while 95% ethanol is used for liquid chromatography. Finally, an exception is made from the non-polar product simulants by performing migration using 3% acetic acid. Acetic acid is used for analytically technical reasons for the chemical analyses of primary aromatic amines (PAA) (see section 3.3) and migration of metals (section 4.2.3). Furthermore, the selection of product simulants is discussed in section 6.2.

3.2 Selection of migration conditions

The migration analyses ought to be carried out over the same period of time as one might expect a product to be contained in packaging and still be for sale. For a cream, this period would typically be 12 months, according to Danish Consumer Council (Forbrugerrådet) [7], but may vary. Since the project duration is limited, it will not be relevant to perform migration for 12 months. Thus, accelerated analyses have been carried out by increasing the temperature, which increases the component migration rate in the PCR matrix.

The selection of temperature and time applied for the simulation of one year can be debated, and it will not be exact science. Within the field of biocides, it is mainly assumed that testing at 54 °C over a period of 14 days simulated the degradation of the product to the same degree as 2-year storage at room temperature.[8] It should be mentioned that it concerns the product itself and not the packaging. In the field of medical equipment, the concept “exhaustive extraction" is applied, which essentially ensures full migration, but it has not been possible to implement it in this project neither based on time-related considerations, nor the aim of this project.

According to the guidelines on migration modelling of relevant substances in plastic articles of PE and PP of the Joint Research Centre of the European Commission, a migration at 60 °C for three days can simulate that the product simulant has been stored in the article for a year (Hoekstra et al., 2015). The Commission Regulation on food contact materials (FCM Regulation (EU) No. 10/2011) suggests 10 days at 60 °C for simulation of 6 months. This may be due to the fact that not only PE/PP is taken into account, and that a safety factor is of importance here as these are food products. For these reasons and since the JRC’s guidelines for theoretical diffusion/migration in plastic matrices (2015) is more recent than the FCM Regulation, a migration time of three days has been applied in this project.

Thus, a migration of three days at 60 °C has been chosen for the PCR plastic samples as appropriate migration conditions for this safety assessment.

[7] https://taenk.dk/test-og-forbrugerliv/sundhed-og-personlig-pleje/tjek-holdbarheden-paa-cremer (accessed on 15 July 2020)

[8] OECD ”guidance document for storage stability testing of plant protection and biocidal products - guidance used in support of pre-registration data requirements for plant protection and biocidal end-use products” (www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO(2015)32&doclanguage=en)

3.3 Prioritization of chemical substances for analysis

Even in virgin plastic, it is possible to find many potentially hazardous substances. In addition to monomers, solvents, impurities, additives, oligomers, and degradation products in virgin plastic, mixing of other materials can take place during use phase and waste phase which can be absorbed in the plastic to be recycled. Researchers have estimated that there are 906 chemicals associated with virgin plastic packaging and additional 3,377 can be possibly included as well. 63 out of those 906 rank highest for hazards to humans and 68 for environmental hazards, when the classification according to CLP[9] is taken into consideration. Additionally, 7 out of 906 are classified as persistent, bio-accumulative and toxic or highly persistent or highly bio-accumulative, and further 15 are classified as endocrine disruptive (Groh et al., 2019). The identified substances are found in plastic as, e.g., monomers, degradation products, solvents, surfactants, softeners, stabilizers, biocides, flame retardants, accelerators, and color agents. PCR plastics can also contain substances that have been absorbed during use, e.g., from cleaning agents, adhesives, labels, and inks, or when mixed with other materials in waste management phase of its lifecycle.

It should be noted that it cannot be ruled out that there is a great variance in the material. It has been previously shown that a great proportion of the substances, measured in number, originate from the lifetime of the plastic at the consumer (Horodytska et al., 2020). Thus, the analysis depends most likely on the specific granules being analyzed. Significant differences in the content of chemical substances can be observed between two analyses of granules performed with a one-month interval measured by quantity and the type of substance. Also, it can be discussed whether the received sample materials are representative for PCR plastics of HDPE and PP on the market. The scope of this problem statement can only be clarified by repeating the study several times and comparing and performing statistical calculations. The variance can be observed from manufacturer to manufacturer, and even from batch to batch.

As it is not possible to analyze all possible chemical substances occurring in samples, this project has chosen to perform three broader screening analyses as well as specific analyses for selected substances/groups of substances. These analyses strategies are described below.

3.3.1 Screening of unknown compounds

The content of unknown chemical compounds, which can migrate into the plastic during the use and lifetime of the plastic, has been assessed to be relevant from the perspective that it is not possible to know the history of plastic. The scientific literature indicates that most chemical substances, which are expected to be detected, originate from the usage of the plastics.

The content of a large part of the problematic substances can be investigated with a GC/MS screening, as this method is suitable for organic components with a boiling point below 500 °C, i.e., a large proportion of the chemical substances that can migrate through the skin barrier. This method is based on gas chromatography (GC) combined with mass spectrometry (MS) and subsequent use of a mass spectrum library, where the identity of the unknown substances in the product simulant can be determined upon assessment. NIST MS data base[10] has been used, which in its most recent edition of 2020 and contains spectra from 306,643 unique compounds. The detection threshold depends directly on the ratio between sample material and product simulant, but by using typical quantities the detection threshold will typically be around 1-100 mg/kg. The uncertainty will be unknown as the response factor between surrogate and

[9] *Classification, Labelling, and Packaging*, Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

[10] Data base of mass spectra from National Institute of Standards and Technology (NIST).

analyte is unknown, and it is recommended that substance-specific analyses are performed for the identified substances which could not be carried out within the framework of this project.

Furthermore, the unknown substances analyzed via LC/MS multitarget analysis, which in principle is not a screening, but a target analysis for many substances. The method is specifically developed for analysis of unknown substances in plastic materials in connection with analysis of food contact materials. It is a liquid chromatographic analysis, which is a better way to examine certain substances (e.g., substances with higher boiling points). This method has also a higher sensitivity than GC/MS screening, but, as it can be seen from component lists for these two methods in Appendix 4 and Appendix 5, there are substances which are covered by both analysis methods. The detection limit for most components is 0.01 mg/kg with an estimated uncertainty of 50 % RSD.

Metals
Migration has been analyzed for 64 different metals using ICP/MS screening. Chromium, cobalt, and nickel are of special interest here, as these may cause contact allergy upon skin contact, according to Asthma-Allergy Denmark (Astma-Allergi Danmark). Also, a screening has been carried out for the content of problematic heavy metals, such as cadmium, mercury, arsenic, and lead, which are undesirable due to their health-related effects. A full list of screened metals can be found in Appendix 6.

Metals are not of interest in relation to fat-based skin cream, and it is not expected that metals can migrate in plastic matrix at a rate that makes them relevant for this project. However, the analysis is considered interesting for more polar products and to be able to compare the obtained analysis results directly with declarations of some manufacturers in the received documentation.

3.3.2 Prioritization of substance-specific analysis

Since it was not possible to analyze all possible chemical substances in the samples, it has been decided in this project to perform three broader screening analyses together with specific analyses for selected substances/groups of substances, which are considered relevant in connection with the subsequent safety assessment of the material. It must be emphasized that the selected substances do not constitute an exhaustive list of substances relevant for analysis in relation to a safety assessment of PCR plastic materials. The selected groups of substances have been described below and prioritized based on the experience and knowledge of the project group:

- Possibly occurring in PCR plastic of PE and PP
- Considered problematic in practice (based on experience)
- Can be absorbed through the skin
- Can be accumulated and/or cause allergenic, immunotoxin, carcinogenic, mutagenic, reprotoxic or endocrine disrupting effects
- Expected to be able to measure with sufficiently low detection limit with available analysis methods.

Polycyclic aromatic hydrocarbons (PAH)
During the recent years, DHI have observed withdrawals of products of recycled plastic due to an increased contact of PAH compounds, most likely due to contaminated black color agent (carbon black). Also, PAHs can be formed by incorrect thermal processing of plastic, and the substance group has been closely observed in the EU. PAHs are carcinogenic upon skin contact, which is why this substance group is relevant for analyses (Straif et al., 2005), (Brf, 2010).

The analysis performed with GC/MC with substance-specific calibration. The analyses were carried out for 15 different PAHs, which were selected on the basis of available standards and run-in methods in the performing laboratory. The list of the specific PAHs is shown in TABLE

17. The analysis has been performed on the product simulant – isooctane. The detection limit is 0.2 mg/kg per component with an estimated uncertainty of 15 %RSD.

Primary aromatic amines (PAAs)
Primary aromatic amines are not expected to be found in a fraction of virgin plastic, but in the recent years a withdrawal of food contact materials of recycled plastic has been observed due to the content of substances. PAA are thought to originate from materials that are joined with polyurethane adhesives (PU adhesive) or by heating with water (Campanella et al., 2015). PAA is considered as carcinogenic and is thus subject to specific restrictions, e.g., in legislation on food contact materials.

The LC/MS analysis was performed on 21 different PAAs selected according to CMR properties. The list of specific PAAs is found in TABLE 18. Due to analytically technical reasons, the analysis for PAAs has been carried out with 3 % acetic acid as product simulant and a detection limit 2 µg/kg product simulant, and with an estimated uncertainty of 20 % RSD.

Potential degradation products of antioxidants and stabilizers
Experience shows that degradation products of stabilizers and antioxidants (often referred to as PE-phenols, even though the group also includes substances without phenol structure) migrate out of PE plastic (and PP plastic) and can be measured in drinking water from water pipes. The group of substances includes substances that may damage liver and kidneys and are also suspected to cause genetic damage (Miljøstyrelsen, 2007).

All plastics are added antioxidants and other stabilizers to stabilize the plastic against degradation during processing and against, e.g., sun and other oxidative stresses. When recycling plastic, it is melted at approx. 200 °C, so that additional stabilizers can be added to avoid material degradation. Both stabilizers and their degradation products can diffuse (move) in the plastic and thus they can also escape the plastic. Stabilizers are usually so large that cannot move very fast, but their degradation products are smaller and thus it is relevant to analyze for these substances.

The potential degradation products are analyzed using GC/MS with substance-specific calibration. 15 different degradation products have been analyzed, which are selected according to available standards and run-in methods in the performing laboratory. The list of specific degradation products (PE-phenols) is shown in TABLE 19. The analysis has been performed with the product simulant isooctane. The detection limit is 0.2 mg/kg product simulant, and with an estimated uncertainty of 15 % RSD.

Perfluoroalkyl and polyfluoroalkyl substances (PFAS)
Even though PFAS are normally not included in PE and PP, they may be adsorbed from mixing with PFAS-treated textile, cardboard for food packaging and plastic. Perfluoroalkyl and polyfluoroalkyl substances are considered relevant in this context because PFAS can have a range of reprotoxic, immunotoxin, persistent and neurotoxic effects. It has been specifically shown that PFAS in humans are associated with impaired immune response to vaccines (EFSA, 2020). PFAS have been previously shown to be able to be absorbed by up to 70 % through the skin (Brinch et al., 2018; Franko et al., 2012).

The presence of PFAS has been examined as a component-specific content analysis using tandem mass spectrometry (LC/MS/MS). 22 different PFAS have been analyzed according to available standards and run-in methods in the performing laboratory. The list of specific PFAS is shown in TABLE 20. The detection limit is 0.005 mg/kg. This has been assessed to be sufficient as the tolerable intake is 8 ng/kg bw/week (EFSA, 2020), but the limit for cosmetic packaging is expected to be higher than for food contact materials.

As it is not possible to analyze the content of all perfluoroalkyl and polyfluoroalkyl substances, the analysis has been supplemented with the measurement of total fluorine. This provides an indication of whether large amounts of fluorine are present, and whether perfluoroalkyl and polyfluoroalkyl substances can still be present in the material. Fluoride is generally not used as additive or anything else in the material, and the presence of fluorine will thus most likely be related to inadequate sorting or originate from perfluoroalkyl and polyfluoroalkyl substances. The analysis of total fluorine is based on a controlled combustion and subsequent ion chromatography, which has been described in Appendix 3.8 and follows EN 14582:2016 with an expected detection limit of 20 mg/kg, and an estimated uncertainty of 15 % RSD.

3.4 Summary of analysis program

Based on the description in sections 3.1-3.3, the analysis program of this project can be summarized as shown in TABLE 6.

TABLE 6 Summary of analysis program.

Analyzed substances	Analysis method	Product simulant (migration in 3 days, 60 °C)	Number of samples
(Screening)	GC/MS	Isooctane	7
(Multitarget-analysis), see Appendix 3.3	LC/MS	95 % ethanol	7
(Screening of) selected metals	ICP/MS	3 % acetic acid	4
PAH	GC/MS	Isooctane	4
PAA	LC/MS/MS	3 % acetic acid	4
PE-phenols (degradation products of antioxidants and stabilizers)	GC/MS	95 % ethanol	7
Perfluoroalkyl and polyfluoroalkyl substances (PFAS)	LC/MS/MS	(Content analysis)	4
Total content, fluoride	EN 14582:2016	(Content analysis)	4

4. Chemical analyses

This chapter presents the performance and results of migration studies and chemical analyses of selected samples (TABLE 5) according to the analysis program shown in TABLE 6. Further information on applied analyses methods can be found in Appendix 3.

4.1 Migration

Migration and analysis have been performed on seven selected samples. Migrations were carried out with a ratio of 1:1 between mass and liquid (approx. 1 g sample material per mL migration liquid). Migrations were run for 72 hours (3 days) at 60 °C, after which the liquid was removed and taken for further analysis. A detailed overview of migration conditions is described in Appendix 2.1

A relatively large amount of sample materials was used during migration (plastic granules) according to product simulant. It has been estimated that in many real cases the amount of the cosmetic product will be larger according to packaging, which is why this part of the analysis can be considered as 'worst case' and may for the basis for further calculations for specific packaging/product-ratio.

Appendix 2.2 shows that organic product simulants (isooctane and 95 % ethanol) have acquired the color of the plastic material in samples 3.5, 4.2 and 5.3 during migration. This is expected to happen when using plastic for packaging of fat-containing products. However, it is unknown which substances are the cause of this color.

4.2 Screening analyses

This section presents the results of three different types of screening analyses. The two broader screenings (GC/MS and LC/MS) have been performed on 7 selected PCR plastic samples, while metal screenings (ICP/MS) are performed on 4 out of these samples.

4.2.1 GC/MS screenings

GC/MS screening investigates substances whose presence in a sample is unknown in advance. The analysis is performed and later an attempt is made to identify those substances which send a response in the analysis. This makes the analysis suitable for examining products with a content which is unknown in advance, but this also means that the uncertainty of this method is unknown as no component-specific calibration is performed. The analysis is targeted towards organic non-polar and slightly polar substances with a boiling point between approx. 80 and 500 °C, also described as volatile and semi-volatile organic substances. GC/MS screening has been carried out on the 7 selected samples after migration to the product simulant isooctane for 3 days at 60 °C.

The full GC/MS screenings are shown in Appendix 4 and an overall overview is shown in TABLE 7 below. Many substances have been found, and a great part of these substances are non-aromatic aliphatic compounds, which are predominantly alkanes and alkenes and a smaller number of terpenes. The presence of alkanes and alkenes can be explained by the degradation of the primary polymer chain during the lifetime of the plastic.

TABLE 7 Main results from GC/MS screenings of 7 samples. The results are shown as mg analyte per kg product simulant.

Sample No	Total detected* [mg/kg solvent]	Total number of detected components	Non-aromatic aliphatic components* [mg/kg]	Number of non-aromatic aliphatic component
1.1	2.100	41	1.400	14
2.1	7.700	48	7.300	31
3.3	4.000	69	3.200	32
3.5	3.700	95	2.600	33
4.2	2.300	57	720	45
5.3	5.700	116	5.100	94
5.4	980	30	530	15

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 8 to TABLE 14 show substances that are tentatively identified in different samples. The tables do not include non-aromatic aliphatic compounds, as these are found in large amounts and behave relatively similarly.

Saturated non-aromatic aliphatic compounds are also referred to as MOSH (mineral oil saturated hydrocarbons). The full screenings including non-aromatic aliphatic compounds and unidentified or partially identified components are shown in Appendix 4. For a final positive identification, a substance-specific analysis with reference substances must be performed, which is not included in this project.

TABLE 8 Identified components in product simulant (isooctane) from the migration of sample no. 1.1, except non-aromatic aliphatic compounds. The results are shown as mg analyte per kg product simulant.

Component (sample no. 1.1)	RT [min]	CAS No.	Concentration* [mg/kg]
1-Butoxy-2-propanol	6,748	5131-66-8	5.8
Methyl dihydrojasmonate	10,818	24851-98-7	5
n-Hexyl salicylate	11,017	6259-76-3	42
α-Hexylcinnamaldehyde	11,519	101-86-0	21
Isopropyl myristate	11,572	110-27-0	43
Hexadecanoic acid, methyl ester	12,337	112-39-0	11
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,605	82304-66-3	11
Isopropyl palmitate	13,018	142-91-6	44
Methyl stearate	13,914	112-61-8	4.3
Octadecenoic acid ethyl ester	14,274	6114-18-7	4.2
Tributyl acetyl citrate	14,937	77-90-7	4.5
Octan-2-yl palmitate	17,011	55194-81-5	4.2
Bumetrizole	18,267	3896-11-5	34
Octocrylene	18,739	6197-30-4	7
Squalene	19,440	111-02-4	7.8
Tris-(2,4-di-t-butylphenyl) phosphite	23,569	31570-04-4	110

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 9 Identified components in product simulant (isooctane) from migration of sample no. 2.1 except non-aromatic aliphatic compounds. Results are shown as mg analyte per kg product simulant.

Component (sample no. 2.1)	RT [min]	CAS No.	Concentration* [mg/kg]
Limonene	7,380	138-86-3	15
2-Propylheptanol	8,340	10042-59-8	16
3-Methyltridecane	9,065	6418-41-3	4.3
2,4-Di-tert-butylphenol	9,868	96-76-4	6.9
n-Hexyl salicylate	11,017	6259-76-3	16
α-Hexylcinnamaldehyde	11,519	101-86-0	8.8
Isopropyl myristate	11,572	110-27-0	20
Hexadecanoic acid, methyl ester	12,337	112-39-0	9.3
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,609	82304-66-3	32
Isopropyl palmitate	13,023	142-91-6	13
Methyl stearate	13,914	112-61-8	3.9
Bumetrizole	18,262	3896-11-5	15
Squalene	19,440	111-02-4	4.6
Tris-(2,4-di-t-butylphenyl) phosphite	23,569	31570-04-4	140

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 10 Identified components in product simulant (isooctane) from migration of sample no. 3.3 except non-aromatic aliphatic compounds. Results are shown as mg analyte per kg product simulant.

Component (sample no. 3.3)	RT [min]	CAS No.	Concentration* [mg/kg]
α-Pinene	6,723	80-56-8	6.4
Limonene	7,380	138-86-3	24
o-Cymene (or isomer)	7,994	527-84-4	6.9
Isophorone	8,086	78-59-1	3.8
1-Decanol	8,651	112-30-1	30
tert-Butyl cyclohexyl acetate	8,846	88-41-5	11
2,4-Di-tert-butylphenol	9,873	96-76-4	24
Butylated hydroxytoluene	9,885	128-37-0	10
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB)	10,302	6846-50-0	7.0
Diethyl phthalate	10,448	84-66-2	35
Octyl ether	10,589	629-82-3	17
Methyl (3-oxo-2-pentylcyclopentyl)acetate (hedione)	10,818	24851-98-7	9.4
α-Hexylcinnamaldehyde	11,519	101-86-0	23

Component (sample no. 3.3)	RT [min]	CAS No.	Concentration* [mg/kg]
Isopropyl myristate	11,572	110-27-0	43
Benzyl benzoate	11,752	120-51-4	5.9
2-Ethylhexyl salicylate	11,816	118-60-5	5.6
Versalide	12,161	88-29-9	21
Hexadecanoic acid, methyl ester	12,342	112-39-0	21
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,609	82304-66-3	9.1
Isopropyl palmitate	13,023	142-91-6	39
Methyl elaidate (double bond may be different position)	13,758	112-62-9	14
Methyl stearate	13,919	11261-8	4
Oxybenzone	14,002	131-57-7	7.4
Ethyl oleate	14,279	111-62-6	13
Octinoxate	16,017	5466-77-3	64
Octan-2-yl palmitate	17,020	55194-81-5	19
Bis(2-ethylhexyl) phthalate (DEHP)	17,497	117-81-7	42
Dodecanoic acid, dodecyl ester	17,590	13945-76-1	6.5
Bumetrizole	18,267	3896-11-5	5.8
Octocrylene	18,744	6197-30-4	11
Hexadecanoic acid, decyl ester	19,133	42232-27-9	22

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 11 Identified components in product simulant (isooctane) from migration of sample no. 3.5 except non-aromatic aliphatic compounds. Results are shown as mg analyte per kg product simulant.

Component (sample no. 3.5)	RT [min]	CAS No.	Concentration* [mg/kg]
tert-Butyl cyclohexyl acetate	8,846	88-41-5	6.5
2,4-Di-tert-butylphenol	9,868	96-76-4	4
Octyl ether	10,589	629-82-3	10
n-Hexyl salicylate	11,017	6259-76-3	25
5-Phenyldodecane	11,095	2719-63-3	2.7
4-Phenyldodecane	11,197	2719-64-4	4.8
Isopropyl myristate	11,572	110-27-0	20
2-Phenyldodecane	11,655	2719-61-1	4.5
6-Phenyltridecane	11,689	4534-49-0	4.3
5-Phenyltridecane	11,752	4534-50-3	3.8
2-Ethylhexyl salicylate	11,821	118-60-5	6.5
4-Phenyltridecane	11,864	4534-51-4	3.8
1-Hexadecanol	12,074	36653-82-4	60
Versalide	12,166	88-29-9	7.5
Hexadecanoic acid, methyl ester	12,342	112-39-0	6.7

Component (sample no. 3.5)	RT [min]	CAS No.	Concentration* [mg/kg]
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,609	82304-66-3	17
Isopropyl palmitate	13,028	142-91-6	53
Methyl stearate	13,914	112-61-8	6,8
Ethyl oleate	14,279	111-62-6	24
Octanoic acid, dodecyl ester	14,328	20292-09-5	7,6
Oleamide (may be different chain length)	14,635	301-02-0	3,5
Co-elution, Tributyl acetyl citrate and saturated alkane	14,941	77-90-7	3,9
n-Propyl 11-octadecenoate	15,092	1000336-71-7	20
Oleamide (may be different chain length)	16,222	301-02-0	50
Piperonyl butoxide	16,689	51-03-6	2,8
Octan-2-yl palmitate	17,020	55194-81-5	22
Diethylhexyl phthalate (DEHP)	17,497	74746-55-7	14
Dodecanoic acid, dodecyl ester	17,590	13945-76-1	84
Bumetrizole	18,272	3896-11-5	18
Octocrylene	18,749	6197-30-4	23
Tetradecanoic acid, dodecyl ester	19,114	2040-64-4	45
Squalene	19,445	111-02-4	4,8
Hexadecanoic acid, dodecyl ester	20,535	42232-29-1	35
Tris-(2,4-di-t-butylphenyl) phosphite	23,559	31570-04-4	22

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 12 Identified components in product simulant (isooctane) from migration of sample no. 4.2 except non-aromatic aliphatic compound. Results are shown as mg analyte per kg product simulant.

Component (sample no. 4.2)	RT [min]	CAS No.	Concentration* [mg/kg]
2,6-Di-tert-butylbenzoquinone	9,800	719-22-2	27
2,4-Di-tert-butylphenol	9,868	96-76-4	84
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	11,655	1620-98-0	16
Methyl 3-(3,5-di-tert-butyl-4-hydroxy-phenyl)propionate	12,565	6386-38-5	14
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,638	82304-66-3	310
Bis(2-ethylhexyl) phthalate (DEHP)	17,497	117-81-7	44
Tris-(2,4-di-t-butylphenyl) phosphite	23,612	31570-04-4	1000

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 13 Identified components in product simulant (isooctane) from migration of sample no. 5.3 except non-aromatic aliphatic compounds. Results are shown as mg analyte per kg product simulant.

Component (sample no. 5.3)	RT [min]	CAS No.	Concentration* [mg/kg]
3,5,5-Trimethyl-2(5H)-furanone	9,002	50598-50-0	6.8
Co-elution, aliphatic compound and 2,4-Di-tert-butylphenol (CAS: 96-76-4)	9,868	(96-76-4)	160
Butylated hydroxytoluene	9,907	128-37-0	51
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,624	82304-66-3	81
Tetraethylene glycol di-2-ethylhexoate	16,83	18268-70-7	7.3
Bis(2-ethylhexyl) phthalate (DEHP)	17,507	117-81-7	10

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

TABLE 14 Identified components in product simulant (isooctane) from migration of sample no. 5.4 except non-aromatic aliphatic compounds. Results are shown as mg analyte per kg product simulant.

Component (sample no. 5.4)	RT [min]	CAS No.	Concentration* [mg/kg]
Limonene	7,380	138-86-3	6.8
2,4-Di-tert-butylphenol	9,868	96-76-4	37
Butylated hydroxytoluene	9,897	128-37-0	5.8
Hexadecanoic acid, methyl ester	12,336	112-39-0	6.9
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12,604	82304-66-3	11
Ethyl oleate	14,255	111-62-6	9.7
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (DEHP)	17,488	74746-55-7	8.4
Tris-(2,4-di-t-butylphenyl) phosphite	23,559	31570-04-4	3.8

*: Concentration has been indicated as naphthalene equivalent. See Appendix 3 for detection limits and method descriptions.

4.2.2 LC/MS multitarget analyses

The LC/MS multitarget analysis is a method developed to examine plastic materials intended for food contact for the migration of undesired components. 110 specific compounds are examined. Only the detected components are reported. A full list of the examined components is shown in Appendix 5. LC/MS multitarget analyses has been performed on migration to product simulant 95 % ethanol after a 3-day migration at 60 °C. The analyses are performed on the 7 selected PCR plastic samples.

TABLE 15 . Identified components in LC/MS multitarget analysis in product simulant (95 % ethanol) from migration. Results are shown as mg analyte per kg product simulant.

Component	CAS No.	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.3 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 4.2 Migrated amount [mg/kg]	Sample 5.3 Migrated amount [mg/kg]	Sample 5.4 Migrated amount [mg/kg]
3,3'-Dichlorobenzidine	91-94-1	-	0.007	0.035	0.099	-	-	-
4-Chloro-o-toluidine	95-69-2	-	-	0.014	0.037	-	-	-
2.4-Diaminotoluene	95-80-7	-	-	-	0.006	-	-	-
4,4'-Diaminodiphenylmethane	101-77-9	-	0.006	0.623	0.038	-	-	-
p-Chloroaniline	106-47-8	-	-	-	0.022	-	-	-
o-Toluidine	95-53-4	0.007	0.027	0.042	0.45	-	-	-
o-Ansidine	90-04-0	-	0.005	0.014	0.64	0.004	0.041	-
Benzoguanamine	91-76-9	-	-	-	0.63	-	-	-
Benzophenone	119-61-9	1.2	0.587	2.2	0.25	-	-	0.58
2-Methylbenzophenone and/or 4-methylbenzophenone	131-58-8 134-84-9	0.42	0.26	0.55	0.41	-	-	0.33
Methyl-2-benzoylbenzoate (MBB)	606-28-0	0.43	0.22	0.021	0.22	-	-	-
4-Phenylbenzophenone	2128-93-0	0.97	0.62	0.21	2.8	-	-	-
2-Isopropylthioxanthone (2-ITX)	5495-84-1			0.17	0.040	-	-	-
Ethyl 4-dimethylaminobenzoate	10287-53-3	0.082	0.047	0.016	0.019	-	-	-
2-Ethylhexyl-4-(dimethylamino)benzoate	21245-02-3	0.24	0.054	0.033	0.28	-	-	-
2-Methyl-4'-(methylthio)-2-morpholinopropiophenone	71868-10-5	-	-	0.042	-	-	-	-
2,4-Diethyl-9H-thioxanthen-9-one	82799-44-8	0.11	0.068	0.033	0.25	-	-	0.017
Ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate	84434-11-7			-	0.016	-	-	-
1,6-Hexanediol diacrylate (HDDA)	13048-33-4	0.40	0.019	-	-	-	-	-
Trimethylolpropane triacrylate	15625-89-5	0.025	-	-	-	-	-	-
Tri(propylene glycol) diacrylate	42978-66-5	0.14	-	-	-	-	-	-
Diethylphthalate	84-66-2	0.28	0.18	12	0.17	0.015	0.24	0.43
Diisobutylphthalate	84-69-5	0.11	0.29	0.38	0.89	0.29	6.6	0.57
Dibutylphthalate	84-74-2	0.098	0.14	7.8	0.54	0.24	4.5	1.8

Component	CAS No.	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.3 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 4.2 Migrated amount [mg/kg]	Sample 5.3 Migrated amount [mg/kg]	Sample 5.4 Migrated amount [mg/kg]
Benzylbutylphthalate	85-68-7			-	0.43	-	-	-
Dibutyl sebaccate	109-43-3	0.18	0.62	-	0.26	-	-	0.021
Tributyl citrate	77-94-1	0.066	0.028	-	0.21	-	0.016	0.016
Tributyl O-acetylcitrate	77-90-7	0.69	0.20	0.021	0.65	-	-	0.057
Salicyclic acid	69-72-7	-	0.048	0.102	0.21	-	-	-
2-Hydroxy-4-methoxy benzophenone	131-57-7	0.70	0.33	4.4	0.17	-	0.093	0.064

-: The result is below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.2.3 ICP/MS screening

An overall impression of migratory metals from the PCR materials is given using ICP/MS screening after 3-day migration to the product simulant 3% acetic acid. Thereafter, the content of 65 different metals has been investigated. Only the detected metals are shown below. The complete list of investigated metals can be found in Appendix 6. ICP/MS screenings are performed on 4 selected PCR plastic samples.

TABLE 16 . Identified components in ICP/MS screening of the product simulant (3 % acetic acid) from the migration. Results are shown as mg analyte per kg product simulant.

Metal	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 5.4 Migrated amount [mg/kg]
Sodium	1.2	-	2.2	7.0
Magnesium	0.11	-	0.30	0.41
Aluminum	-	0.46	0.49	0.60
Potassium	1.2	-	-	0.14
Calcium	0.43	0.10	2.7	4.1
Manganese	-	-	-	0.01
Iron	0.15	-	0.28	0.18
Copper	0.02	-	0.05	-
Zinc	0.08	-	0.18	0.09
Strontium	-	-	0.07	0.02
Barium	-	-	0.29	-

-: The result is below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.3 Component-specific analyses

Selected component-specific analyses of selected PCR samples have been performed after migration to the applied product simulants. The component-specific analyses have been selected during an initial process (see section 3.3.2) and have a relatively low detection limit compared to screening analyses.

4.3.1 Polycyclic aromatic hydrocarbons (PAH)

Selected PAH compounds have been investigated. The analysis has bene performed on 7 selected PCR plastic samples after a 3-day migration at 60 °C to the product simulant isooctane.

TABLE 17 Results for the content of PAH compounds in product simulant (isooctane) from migration. Results are shown as mg analyte per kg product simulant.

Component	CAS No.	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.3 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 4.2 Migrated amount [mg/kg]	Sample 5.3 Migrated amount [mg/kg]	Sample 5.3 Migrated amount [mg/kg]
Naphthalene	91-20-3	-	-	4.4	-	-	1.1	0.24
Acenaphtene	83-32-9	-	-	0.14	-	-	0.52	-
Acenaphtylene	208-96-8	-	-	-	-	-	-	-
Phenanthrene	85-01-8	0.31	-	0.69	0.47	0.17	6.2	0.92
Anthracene	120-12-7	-	-	0.21	-	-	1.7	-
Fluorene	86-73-7	-	-	0.36	-	-	0.83	0.16
Fluoranthene	206-44-0	-	-	0.28	-	0.24	1.6	0.22
Pyrene	129-00-0	-	-	0.34	-	0.16	0.88	0.15
Benzo(a)anthracene	56-55-3	-	-	-	-	-	-	-
Chrysene, triphenylene	218-01-9, 217-59-4	-	-	-	-	-	-	-
Benzo[b]fluoranthene, Benzo[j]fluoranthene, Benzo[k]fluoranthene	205-99-2, 205-82-3, 207-08-9	-	-	-	-	-	-	-
Benzo(a)pyrene, Benzo(e)pyrene, perylene	50-32-8, 192-97-2, 198-55-0	-	-	-	-	-	-	-
Indeno(1,2,3-cd)pyrene	193-39-5	-	-	-	-	-	-	-
Dibenzo[a,h]anthracene	200-181-8	-	-	-	-	-	-	-
Benzo[ghi]perylene	191-24-2	-	-	-	-	-	-	-

-: The result is below detection limit for applied method. See Appendix 3for detection limits and method descriptions.

4.3.2 Primary aromatic amines (PAA)

Selected PAA compounds have been investigated. The analysis has been performed on 4 selected PCR plastic samples after a 3-day migration at 60 °C the product simulant 3 % acetic acid.

TABLE 18 Results of PAA compound content in product simulant (3 % acetic acid) from migration. The results are shown as mg analyte per kg product simulant.

PAA compound	CAS No.	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 5.4 Migrated amount [mg/kg]
2,4,5-Trimethylaniline	88-05-1	-	-	-	-
2,4-Diaminoanisole	615-05-4	-	-	0.015	-
2,4-Diaminotoluene	95-80-7	-	-	-	-
2-Methoxyaniline	90-04-0	-	-	0.54	-
2-Naphthylamine	91-59-8	-	-	-	-
3,3'-Dichlorobenzidine	91-94-1	-	-	0.005	-
3,3'-Dimethoxybenzidine	119-90-4	-	-	-	-
3,3'-Dimethylbenzidine	612-82-8	-	-	-	-
3,3'-Dimethyl-4,4'-diaminodiphenylmethane	838-88-0	-	-	-	-
4,4'-Diaminodiphenylmethan	101-77-9	0.003	0.005	0.026	0.002
4,4'-Methylen-bis-2-chloranilin	101-14-4	-	-	-	-
4,4'-Oxydianilin	101-80-4	-	-	-	-
4,4'-Thiodianilin	139-65-1	-	-	-	-
4-Aminoazobenzen	60-09-3	-	-	-	-
4-Aminobiphenyl	92-67-1	-	-	-	-
4-Chloroanilin	106-47-8	-	-	-	-
4-Chlor-o-toluidin	95-69-2	-	-	0.025	-
Benzidin	92-87-5	-	-	-	-
o-Aminoazotoluen	97-56-3	-	-	-	-
o-Toluidin	95-53-4	0.007	0.021	0.54	0.002
p-Cresidin	120-71-8	-	-	-	-

-: The results are below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.3.3 Degradation products of stabilizers and antioxidants (PE-phenols)

Selected PE-phenols have been investigated. Analysis has been performed on 7 selected PCR plastic samples after a 3-day migration at 60 °C to the product simulant 95 % ethanol.

TABLE 19 Results on the content of PE-phenols in product simulant (95 % ethanol) from the migration. Results are shown as mg analyte per kg product simulant.

PE-phenol component	CAS No.	Sample 1.1 Migrated amount [mg/kg]	Sample 2.1 Migrated amount [mg/kg]	Sample 3.3 Migrated amount [mg/kg]	Sample 3.5 Migrated amount [mg/kg]	Sample 4.2 Migrated amount [mg/kg]	Sample 5.3 Migrated amount [mg/kg]	Sample 5.4 Migrated amount [mg/kg]
Acetophenone	98-86-2	-	-	0.22	-	-	-	-
5-Methyl-2-hexanone	110-12-3	-	-	-	-	-	-	-
4-Ethylphenol	123-07-9	-	-	-	-	-	1.2	-
4-tert-Butylphenol	98-54-4	-	-	-	-	0.10	0.12	-
4-Butoxyphenol	122-94-1	-	-	0.08	-	-	-	-
2,6-Di-tert-butyl-1,4-benzoquinone	719-22-2	-	-	1.1	1.6	48	11	-
2,4-Di-tert-butylphenol	96-76-4	-	2.2	4.1	2.0	4.5	6.5	4.6
2,6-Bis(1,1-dimethyl)-4-methylphenol	128-37-0	0.33	0.38	1.7	0.67	-	5.9	2. 4
3,5-Di-tert-butyl-4-hydroxystyrene	52858-87-4	-	-	0.15	0.42	0.44	0.69	0.14
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0	0.13	0.32	0.69	0.72	4.6	0.72	0.39
3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	-	-	-	-	0.70	-	-
7,9-Di-tert-butyl-1-oxaspiro(4,5)decra-6,9-diene-2,8-dione	82304-66-3	1.3	4.1	1.1	4.7	26	4.3	2.0
3-Methyl-3,5-di-tert-butyl-4-hydroxyphenylpro-panoate	6386-38-5	0.24	0.80	0.26	0.49	-	0.28	0.25
3,5-Di-tert-butyl-4-hydroxybenzoic acid	1421-49-4	-	-	-	-	-	-	-
3,5-Di-tert-butyl-4-hydrophenyl propionic acid	20170-32-5	-	-	-	-	-	-	-

-: The results are below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.3.4 Perfluoroalkyl and polyfluoroalkyl substances (PFAS)

The content of selected PFAS in the sample materials has been investigated. This analysis has been performed as a content analysis and not as a migration analysis, which is the case for most of the other analyses.

TABLE 20 Results for PFAS content in the selected PCR samples. This is a content analysis. Results are shown as mg analyte per kg sample material.

PFAS component	CAS No.	Sample 1.1 Total amount [mg/kg]	Sample 2.1 Total amount [mg/kg]	Sample 3.5 Total amount [mg/kg]	Sample 5.4 Total amount [mg/kg]
Perfluorooctacte sulfonate (PFOS)	45298-90-6	-	-	-	-
Perfluorooctanoic acid	335-67-1	-	-	-	-
Perfluorobutansulfonate (PFBS)	375-73-5	-	-	-	-
Perfluorobutanoic acid (PFBA)	375-22-4	-	-	-	-
Perfluoropentane acid (PFPeA)	2706-90-3	-	-	-	-
Perfluorohexane sulfonate (PFHxS)	355-46-4	-	-	-	-
Perfluorohexanoic acid (PFHxA)	307-24-4	-	-	-	-
Perflyuoroheptane sulfonate (PFHpS)	375-92-8	-	-	-	-
Perfluoroheptanoic acid (PFHpA)	375-85-9	-	-	-	-
Perfluorooctane-sulfonamide	754-91-6	-	-	-	-
Perfluorononanoic acid (PFNA)	375-95-1	-	-	-	-
Perfluoro decane sulfonate	67906-42-7	-	-	-	-
Perfluorodecanoic acid (PFDA)	335-76-2	-	-	-	-
Perfluoroundecanoic acid (PFUnA)	2058-94-8	-	-	-	-
Perfluorododecanoic acid (PFDoA)	307-55-1	-	-	-	-
Perlfuorotridecanoic acid	376-03-4	-	-	-	-
Perfluorotetradecanoic acid	376-06-7	-	-	-	-
Perfluoro-3,7-dimethyloctanoic acid (PF-3,7-DMOA)	172155-07-6	-	-	-	-
7H-dodecafluoroheptanoic acid (HPFHpA)	1546-95-8	-	-	-	-
6:2 Fluorotelomer sulfonate	27619-97-2	-	-	-	-
4:2 Fluorotelomer sulfonate	757124-72-4	-	-	-	-
8:2 Fluorotelomer sulfonate	39108-34-4	-	-	-	-

-: The results are below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.3.5 Total fluoride content

The total fluoride content was determined after controlled combustion with subsequent ion chromatography. The method follows EN 14582:2016 (as described in 82) and just like the PFAS analysis it is a content analysis, not a migration analysis.

TABLE 21 Results of total fluoride content in the selected PCR samples. This is a content analysis. Results are shown as mg analyte per kg sample material.

Component	Sample 1.1 Total amount [mg/kg]	Sample 2.1 Total amount [mg/kg]	Sample 3.5 Total amount [mg/kg]	Sample 5.4 Total amount [mg/kg]
Total fluoride	-	-	-	-

-: The results are below detection limit for applied method. See Appendix 3 for detection limits and method descriptions.

4.4 Summary of analysis results

The performed analyses have revealed a high number of components. It has also been observed that some PCR samples discolor the product simulant, which means that the PCR plastic, if used in packaging, potentially can discolor the cosmetic products, and thus change its visual appearance.

The GC/MS screening has detected a high number of non-aromatic aliphatic compounds, where the majority are found to be saturated. The non-aromatic, saturated aliphatic compounds may possibly originate from the degradation of a polymer chain. The component type is present to a high degree, and is the largest group detected. The content of these components in the samples is semi-quantitatively determined to be between 530 mg/kg and 7,300 mg/kg (corresponding to 0.05 % and 0.7 %, respectively).

Table 7 provides an overview of the components found in the GC/MS screening. The total number of analyzable organic substances varies from 980 mg/kg to 7,700 mg/kg. The majority of these substances is constituted by non-aromatic aliphatic compounds. These are linear or branched aliphatic compounds, and their origin is unknown. It is striking that these compounds are observed in all samples, and it can be speculated whether it is the degradation of the primary polymer chain since this is constituted of the same chemical compound (polyolefins). Some PCR plastic samples contain more components than others, and a large difference can be seen in the amount of non-aliphatic components. This group includes, e.g., additives, degradation products of additives and substances that can be absorbed or adsorbed during the lifetime of the plastic, e.g., while being at the consumer.

Sample no. 3.5 also contains several aromatic compounds of aliphatic functionality (MOAH, mineral oil aliphatic hydrocarbons), such as 5-phenyltridecane. These do not originate from the degradation of the polymer chain, which does not have an aromatic functionality, and may be, for example, components that have migrated into plastic during its lifetime while being used by the consumer.

Furthermore, many different esters and terpenes have been found, which may have an impact on the olifactory properties. Here, it is possible to mention limonene, α-hexylcinnamaldehyde and methyl dihydrojasmonate as examples on specific fragrance substances, and isopropylmyristate as a processing aid used in connection with addition of a fragrant substances. The fragrant substance versalide was found in a few samples.

Tris-(2,4-di-tert-butylphenyl)phosphite has been detected in all samples. The component is possibly as an antioxidant during reprocessing of recycled plastic to ensure that the recycled plastic is resistant to oxidation.

Octocrylene has also been found in several samples. The component is most likely added as an UV-filter to protect the plastic material, but this component can also be used as an UV-filter in sunscreen lotions. In the same way, bumetrizole is a plastic additive with function as an UV-filter.

Several examples of degradation products of antioxidants and stabilizers have been found in the substance-specific analyses of these. This corresponds to the results of GC/MS screenings. The most prominent are 2,6-di-tert-butyl-1,4-benzoquinone and 7,9-di-tert-butyl-1-oxaspiro(4,5)decra-6,9-dien-2,8-dione detected in the product simulant in concentrations of 48 and 26 mg/kg, respectively.

Also, the presence of legally (REACH) restricted phthalates, such as DBP, DIBP, BBP and DEHP has been detected in several samples. The content is relatively low (in all cases below 0.005 %) but may have an impact on the product’s access to the market.

The LC/MS multitarget analysis detected a range of different components related to the production of recycled plastic, including softeners and polymerization agents. Softeners are not added to virgin polyolefins but may have occurred as contaminants during the reprocessing of the plastic. Most of the components detected are present at a level of approx. 1 mg/kg in the applied product simulant.

The ICP/MS screening has revealed a small number of metals that have migrated into the product simulant. No content of the metals typically connected to allergy: nickel, chromium and cobalt has been detected. However, the content of approx. 0.5 mg/kg aluminum has been detected in the product simulant for several samples. For most metals screened for, no content above the detection limit has been detected. Thus, no problematic heavy metals such as cadmium, lead, mercury, or arsenic were found.

Several PAH compounds have been detected in the product simulant in an amount which cannot be ruled out as being relevant. REACH (EC 1907/2006, Annex XVII, entry 50) restricts PAH in toys and 'childcare articles', which come into long-term contact with the throat or skin, to 0.5 mg/kg for 8 selected compounds. The articles may not be marketed, according to the same entry, if the content exceeds 1 mg/kg of the eight PAH compounds.

No content or evidence of fluorinated substances was detected by the component-specific analysis or by the analysis for total fluoride content.

5. Safety assessment

This chapter provides a description of the method and execution of safety assessments of selected substances in the PCR plastic samples. First, the main legal framework for safety assessment of cosmetic products will be described. Then, the selection of specific substances for assessment will be described based on the results from the chemical analyses. This is followed by a description of the method for the assessment including the definition of two selected exposure scenarios. Lastly, the safety assessments are described which result in recommendations for acceptable values for content/migration of the selected substances.

5.1 Legislation for safety assessments

EU's Cosmetic Regulation requires that a cosmetic product safety report is prepared for each cosmetic product, which, among others, includes a safety assessment. Hence, the packaging must be safety assessed both on its own and together with the product. In this project, the safety assessment of the packaging includes those substances which can migrate into the packaged product. These can be both substances that are considered prohibited in cosmetic products, and other problematic substances which are not necessarily prohibited.

The safety assessment of the packaging of a cosmetic product is necessary to be able to avoid unacceptable contamination of the cosmetic product inside the packaging. Article 17 of Cosmetic Regulation on "traces of prohibited substances" establishes that "the non-intended presence of a small quantity of a prohibited substance, stemming from impurities of natural or synthetic ingredients, the manufacturing process, storage, migration from packaging, which is technically unavoidable in good manufacturing practice, shall be permitted provided that such presence is in conformity with Article 3".

Article 3 in the Cosmetic Regulation on safety establishes that "a cosmetic product made available on the market shall be safe for human health when used under normal or reasonably foreseeable conditions of use […]'. This may occur, among others, taking into account labelling, e.g., inclusion in the declaration or indication of restrictions of application.

The main purpose of the required safety assessment is thus to assess whether the cosmetic product is safe for the actual use both in terms of the ingredients used and the packaging, thereby uncovering what the "small amount" means in the specific use situation. If the prohibited substances and other occurring substances are accepted, it should be possible to provide evidence that the substances are technically unavoidable in good manufacturing practice, and that the amount in the product is safe for human health.

Prohibited substances are as follows:

- Substances classified as carcinogenic, mutagenic or reprotoxic (CMR) in category 1A, 1B or 2. A substance, which is classified under category 2, may be used in cosmetic products if the Scientific Committee on Consumer Safety (SCCS) of the European Union have reviewed the substance and have found it safe for use in cosmetic products.
- Substances mentioned in Annex II in the Cosmetic Regulation.

Some substances are allowed in cosmetic products, but with a requirement that certain restrictions are followed. These are included in Annex III of the Cosmetic Regulation. This means that some substances may only be used in some types of products and only with a warning label. Furthermore, in some cases REACH (Annex XVII) must be complied with.

In addition to the added substances in the cosmetic product, many other different substances can be released from the packaging, and this must also be assessed whether the resulting concentration of these substances in the product may be considered as safe in relation to its use.

Thus, the required safety assessment covers both chemical substances in the cosmetic product and substances which can migrate into the cosmetic product from the packaging. This project provides safety assessment for the chemical substances from the packaging only, as the focus of this project is to assess PCR plastic for packaging.

5.2 Selection of substances for safety assessment examples

Due to the limitations of this project, it has been necessary to prioritize a small number of the identified chemical substances in the specific safety assessment.

Those substances found in analyses have been reviewed in detail in order to determine whether allergenic substances, CMR-substances or endocrine disrupting substances could be selected directly. This review also included knowledge on substances on the list of prohibited substances in Annex II to the Cosmetic Regulation and REACH (Annex XVII). After this first non-systematic step, a range of substances were left behind, which were not taken into consideration in the subsequent selection principles.

Furthermore, the priority has been given to those substances that are observed to migrate from several of the analyzed PCR samples, and/or occur in concentrations above the permitted thresholds in plastic used as food contact material (FCM). The requirements for FCM are used solely as guidance to when and which substances are relevant to consider, as the Cosmetic Regulation focuses on direct intake of substances and not on the dermal exposure to substances, which is relevant in relation to cosmetic products. Thus, the aim is not to achieve that PCR plastic must be of FCM-quality to be used for safe packaging of cosmetic products.

According to the above-mentioned, the following substances/group of substances have been selected for safety assessment:

- Aluminum has been selected due to the group of children, who have developed an aluminum allergy in connection to vaccination injuries. It is important that parents are able to choose creams, which they can be sure of not containing aluminum to the extent that can cause itching in the children. It has been found that aluminum migrates in three of the PCR plastic samples when using 3 % acetic acid (product simulant) in up to 0.60 mg Al/kg of simulant.
- Phthalates: di-butylphthalate (DBP), butyl-benzyl-phthalate (BBP) and bis(2-ethylhexyl)phthalate (DEHP) have been selected as they occur in many of the analyzed samples. This indicates that there is a diffuse contamination, which technically can be complicated to avoid in PCR plastic (contamination may originate from PVC, adhesive and ink from labels). The selected phthalates are classified as reprotoxic and are considered endocrine disrupting. Since these substances have the same toxicological activity mode (EFSA CEP Panel, 2019), they are assessed together as one substance.
- Benzophenone has been selected due to its occurrence in a concentration above the allowed as stated in the FCM Regulation ((EF) No 10/2011 on the migration from food contact materials). Benzophenone and several benzophenone-derivates occur in most of the samples. The substance has a low tolerable daily intake (TDI) of 0.03 mg/kg bw/day (EFSA CEF Panel, 2009).
- Tris-(2,4-di-t-butylphenyl)phosphite has been selected because it has been found to migrate from almost all PCR samples. In general, it is found in a concentration much higher than the allowed concentration according to FCM Regulation, where it is used as a stabilizer and antioxidant.

- BHT, that is, the substance 2,6-bis(1,1-dimethyl)-4-methylphenol. BHT is an antioxidant, which is permitted in cosmetics, chewing gum and in industrially used frying oil for food production, and is allowed according to FCM Regulation with a specific migration limit (SMG) of 3 mg/kg. BHT is currently under assessment as being endocrine disrupting (ECHA, 2020) and under CoRAP-assessment in France for potential registration as SVHC-substance.[11] BHT has been detected in almost all analyzed PCR plastic samples, and in a concentration of up to 5.9 mg/kg. BHT can also be a degradation product from other antioxidants used in plastic, e.g., PE and PP.
- 2,4-Di-tert-butylphenol has been selected because it is a frequently occurring degradation product of antioxidants in plastic, and because the quality criteria for drinking water are relatively low: 20 µg/L (Miljøstyrelsen, 2007).

Safety assessment limitations

Due to the framework of the project, it was not possible to perform a complete safety assessment of a PCR plastic material. The following limitations are considered to be the most critical:

- The completed analyses are performed on PCR plastic granules and thus not on pre-molded packaging items.
- Specific PCR materials have been selected after purification, and the extent of variance in chemical content from purification to purification and from source to source is unknown.
- The analyses only include substances which have been specifically searched for in this project, hence other problematic substances than those covered here may be present.
- The final packaging may be supplemented with additional stabilizers, antioxidants, and other additives.
- It was only possible to perform assessments on a few of the substances found to migrate from PCR plastic materials.

5.3 Methodology

The safety assessment has been performed based on the results obtained from performed analyses. Calculation examples and recommendations for acceptable values for content/migration of selected substances have been provided. The safety assessment has been based on the existing guidelines for assessment of ingredient substances, which set out exposure amounts and times for different cosmetic products (SCCS, 2018).

As mentioned above, the safety assessment has been performed based on migration studies from PCR plastic granules and from molded packaging, which in terms of migration cannot necessarily be compared with PCR granules. The safety assessment has specifically been based on expert assessments from the EU's scientific committees (primarily SCCS). The data search has also included a search in REACH registration data. The toxicological profile of substances, the critical effect, and the corresponding NOAEL-/LOAEL values for relevant exposure scenarios, primarily through the skin, have been reviewed. TDI or DNEL values were available for substances, hence these have been applied (see descriptions of abbreviated terms in section 1.3).

According to analysis results, exposure scenarios have been calculated for both baby body lotion (representative of worst case exposure to a product which is not rinsed off (leave-on) and for shampoo for adults (a product which is rinsed off, with short-term exposure as a contrast) based product exposure statements in 'Notes of Guidance' (SCCS, 2018) and taking into account the different exposures when using these packaging. Since babies have a very large surface area in relation to body weight, typically a larger amount of product is applied per body

[11] https://echa.europa.eu/documents/10162/9495d950-1dde-91db-66fa-f565ce9a3fda (Accessed on 9 December 2020)

weight for babies compared to adults, which means that babies are more exposed than adults. Baby body lotion can thus be a representative of the sensitive exposure scenario.

The basic data below are taken from SCCS' 'Notes of Guidance for the testing of cosmetic ingredients and their safety (10th edition, 2018).

5.3.1 Scenario: Baby body lotion

TABLE 22 Basic data for baby body lotion (SCCS, 2018)

Description	Parameter	Value
Average body weight, baby	***K***	3.4 kg[12]
Average body height, baby		51,25 cm[12]
Way of exposure		Dermal
Type of exposure		Product cannot be rinsed off (leave-on).
Quantity per application	***G***	1.1
Quantity per skin surface area	G_A	0.5 mg/cm^2 (adult, Table 2A&3; 7.82g/15670 cm^2)
Frequency of application	***F***	1
Surface area per application	***A***	2200 cm^2 (Cato, 2020)
Retention factor	***R***	1
Percutaneous permeation	***P***	Depending on the substance.

Exposure through skin, E_{dermal} (*Dermal exposure*)

$E_{dermal} = (G_A * A * F * R) / K = (0.5 * 2200 * 1 * 1) / 3.4 = 323.5$ mg baby lotion/kg bw/day

5.3.2 Scenarie: Shampoo

TABLE 23 Basic data for shampoo (adults), (SCCS, 2018)

Description	Parameter	Value
Average body weight, adults	***K***	60 kg
Way of exposure		Dermal
Type of exposure		Rinse-off product
Quantity per day, shower gel	G_{SG}	18.67 g/day
Quantity per day, shampoo	G_{SH}	10.46 g/day
Retention factor, shower gel	R_{SG}	0.01
Retention factor, shampoo	R_{SH}	0.01
Percutaneous permeation	***P***	Depending on substance

Exposure through skin, E_{dermal} (Dermal exposure)

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

5.3.3 Calculation of Margin of Safety (MoS)

In the risk assessment of exposure, a margin of safety (MoS) is calculated taking into consideration the differences in absorption between substances. When assessing the MoS value and

[12] Data for average weight and height for a baby is calculated based on tables from WHO, WHO 2006: WHO Child Growth Standards WHO Child Growth Standards 1 year 2 years 3 years 4 years 5 years Length/height-for-age, weight-for-age, weight-for-length, weight-for-height and body mass index-for-age Methods and development (11 November 2006)

whether there is a risk present, uncertainty factors and limitations in relation to analyses results, exposure estimates (including exposure from other sources) and experimental data which form the foundation for NOAEL/LOAEL values have been taken into consideration. TDI or DNEL value is available for selected substances, and a MoS value of 10 can thus be accepted as 10% of TDI are allocated to cosmetic products, so that exposure of humans from other sources can also be allowed (e.g., from drinking water and food products). In the same way, the maximum acceptable concentrations for substances can be calculated as those concentrations that result in a MoS value of 10.

The Margin of Safety is calculated as the ratio between the NOAEL value and the systemic exposure dose (SED), i.e.:

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

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

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

Here, TDI has been used instead of NOAEL, as TDI values are already available for substances.

Some phthalates have already established DNEL values for dermal exposure, and in this case, these have been applied instead of TDI (see TABLE 25).

For substances with no data available on the substance ability to penetrate the skin, a P-value of 1 is applied, which corresponds to that 100% of the substance penetrates the skin. It is a conservative assumption which is used by default until data is available (Miljøstyrelsen, 2020). SCCS' 'Notes of Guidance' have previously used P-value of 1, where permeation through skin was unknown, according to 8th edition of SCCS/1501/12. Since then, it has been changed to a P-value of 0.5, which is the currently used value in (SCCS, 10th edition). However, the substances that migrate from plastic, are often smaller fractions of larger chemical substances and other substances with a lower molecular weight (less than 500 daltons), which means that these can penetrate the skin, according to 8th edition of SCCS/1501/12. Thus, in this project a P-value of 1 has been applied for those substances, where no data are available on the substance's ability to penetrate the skin.

For the calculation, the measured concentration converted into percentage has been applied. Example: 0.58 mg/kg benzophenone has a systemic exposure (SED) of 0.00013 mg/kg bw/day for baby body lotion with P-value of 0.7 and TDI of 0.03 mg/kg bw/day, where MoS is 228:
SED: 0.000058 / 100 x 0.7 x 323.5 mg/kg bw/day = 0.0001313 mg/kg bw/day
MoS: 0.03 mg/kg bw/day / 0.0001313 mg/kg bw/day = 228.

As the MoS value of 228 is higher than 10, the concentration of benzophenone is 0.58 mg/kg and can be thus entirely assured that contamination from packaging for baby body lotion can be accepted.

In addition, the highest concentration, which is safe for use, is calculated, i.e. the concentration that gives a MoS of 10. For benzophenone, the highest acceptable concentration is calculated (in packaging for baby body lotion) to 13 mg/kg, since:
SED: 0.0013 / 100 x 0.7 x 323.5 mg/kg bw/day = 0.00294 mg/kg bw/day
MoS: 0.03 mg/kg bw/day / 0.00294 mg/kg bw/day = 10.

5.4 Assessment of selected substances

5.4.1 Aluminum

In this project, aluminum and aluminum compounds are only assessed for their critical effect upon skin contact, which is allergy. This has been performed despite the fact that SCCS have assessed that aluminum is safe to use as an ingredient in relatively high concentrations in, e.g., deodorants, and do not find that aluminum used this way is allergenic (sensitizing) (SCCS, 2020). Substances which can migrate from packaging are not entirely an actual ingredient that is declared on packaging. However, some consumers are already sensitized (allergic) to aluminum from childhood vaccinations, and these consumers need to know that aluminum is in products to an extent that can trigger their allergy upon skin contact causing rash and itching.

Aluminum, which is found to be released from PCR plastic samples, can be found in many different compounds, but due to analytically technical reasons it is only indicated as aluminum.

In a study of 21 persons of age 23-71, who are allergic towards aluminum, the allergic reaction was observed for content down to 0.63 % of aluminum chloride hexahydrate and 0.77 % of aluminum lactate (see FIGURE 1). Here, 1-2 out of 21 persons had an allergic reaction, which corresponds to 0.07 % aluminum. This means that aluminum concentration must be lower than 0.07 % to avoid allergic reactions in the most sensitive allergy sufferers. This corresponds to 700 mg Al/kg cosmetic product. If a factor 10 is used for uncertainty due to the small number of tested, an acceptable limit of 70 mg/kg cosmetic product is obtained.

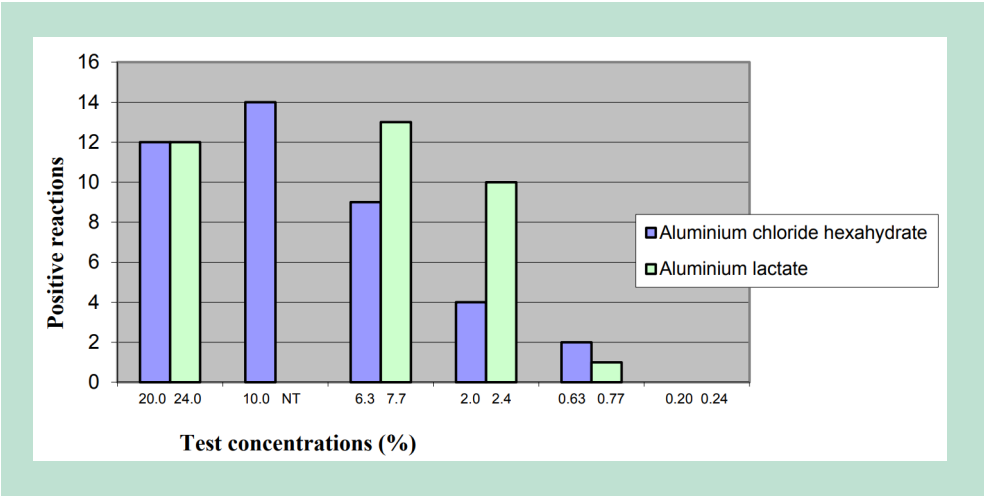

FIGURE 1 Columns show the number of positive reactions to aluminum chloride hexahydrate and aluminum lactate at different equimolar concentrations. NT means ”not tested” (Siemund, et. al, 2012).

Since the highest concentration of aluminum from the four PCR plastic samples analyzed for aluminum is 0.60 mg/kg, it is very far below the proposed acceptable limit. It must be noted that the concentration of aluminum in samples is only measured through an ICP/MS screening, where the uncertainty is unknown.

5.4.2 Phthalates

Since phthalates di-butyl phthalate (DBP), butyl-benzyl-phthalate (BBP) and bis(2-ethylhexyl)phthalate (DEHP) have the same toxicologic activity mode, they are considered as

one. This requires a calculation of a weighted group phthalate concentration[13] expressed as DEHP equivalents, as described by EFSA (EFSA CEP Panel, 2019).

TABLE 24 Harmonized classification of phthalates, occurrence on REACH lists as well as migration limit and other restrictions in FCM Regulation (EU 10/2011).

Name of substance and CAS No.	Harmonized classification (health) and occurrence on REACH lists	SML in FCM Regulation	Cosmetic Regulation
Dibutyl phthalate (DBP), 84-74-2	Repr. 1B H360Df (May damage the unborn child. Suspected of damaging fertility) ED; on candidate list and approval list	0.3 mg/kg. May only be used as: a) softener in recycled materials and objects in contact with non-fatty foods; b) technical auxiliary agent in polyolefins in concentrations at max. 0.05 % in the final product.	On the list of prohibited substances (Annex II)
Benzyl -butyl-phthalate (BBP), 85-68-7	Repr. 1B H360Df (May damage the unborn child. Suspected of damaging fertility) ED; on candidate list and approval list	30 mg/kg. May only be used as: a) softener in recycled materials and objects b) softener in disposable materials and objects in contact with non-fatty foods, except breast milk substitutes and dietary supplement mixtures as defined in Commission Directive 2006/141/EC or processed foods based on cereals and baby food for infants as defined in Directive 2006/125/EC c) technical auxiliary agent in concentrations of max. 0.1 % in the final product.	On the list of prohibited substances (Annex II)
Bis(2-ethylhexyl) phthalate (DEHP), 117-81-7	Repr. 1B H360FD May damage the unborn child. Suspected of damaging fertility) ED; on candidate list and approval list	1.5 mg/kg. May only be used as: a) softener in recycled materials and objects in contact with non-fatty foods; b) technical auxiliary agent in concentrations at max. 0.1 % in the final product.	On the list of prohibited substances (Annex II)

Repr.: Reprotoxic; ED: Endocrine disrupting

As phthalates are classified as reprotoxic, they are prohibited in cosmetic products and are also included on the list of the prohibited substances in the Cosmetic Regulation. The following critical effects are known:

DBP: Reduced sperm count and mammary gland changes in male offspring
BBP: Reduced anogenital distance (feminization in males)
DEHP: Small testicles and prostate as well as testicular atrophy.

TABLE 25 Parameters applied in the safety assessment. NOAEL and TDI from (EFSA CEP Panel, 2019). DNEL from (RAC, 2017).

Name of substance	Skin permeability	NOAEL (mg/kg bw/day)	Oral TDI (mg/kg bw/day)
Di-butyl phthalate (DBP)	0.1 (Andersen, et al., 2012)	LOAEL*: 2	0.1 (DNEL: 0.0067 as internal dose)
Butyl-benzyl-phthalate (BBP)	0.05 (Andersen, et al., 2012)	50	0.5 (DNEL: 0.034 as internal dose)

[13] Phthalate concentration expressed as DEHP equivalents = DEHP*1 + DBP*5 + BBP*0.1 + DINP*0.3

Name of substance	Skin permeability	NOAEL (mg/kg bw/day)	Oral TDI (mg/kg bw/day)
Bis(2-ethylhexyl)-phthalate (DEHP)	0.05 (Andersen, et al., 2012)	4.8	0.05
DBP+BBP+DEHP	0.1 (as worst case)	-	0.05 (expressed as DEHP equivalents)

*LOAEL: Lowest Observed Adverse Effect Level. Used when there has not been a dose group without effects.

The skin permeability of the indicated phthalates is limited. The absorption depends on the esterase activity in the skin, which converts, e.g., dibutyl phthalate (DBP) to monobutyl phthalate, which can then be absorbed in the skin (Sugino et al., 2017).

Based on the allocation of 10 % of TDI for cosmetic products and parameters shown in TABLE 25 and calculated exposure as shown in section 5.3, the highest acceptable concentration can be calculated.

Calculated highest acceptable concentration DEHP equivalents in baby body lotion:
148 mg/kg (results in a MoS value of 10)

Calculated highest acceptable concentration DEHP equivalents in shampoo:
9798 mg/kg (results in a MoS value of 10)

5.4.3 Benzophenone

TABLE 26 Assessment and data applied in the safety assessment of benzophenone.

CAS	119-61-9
Harmonized classification (health) and occurrence on REACH lists	Approved in Risk Assessment Committee in ECHA: Carc 1B; Carcinogenic. Not found on REACH lists.
Cosmetics regulation	Not mentioned but will be prohibited when the approved classification Carc 1B will be implemented.
SML in FCM regulation	0.6 mg/kg food or product simulant.
Skin permeability	0.7 (ECHA, 2019)
NOAEL	Via dermal exposure: LOAEL: 15 mg/kg bw/day (ECHA, 2020). BMDL10: 3.1 mg/kg bw/day, Critical effect: non-neoplastic effects in kidneys. (EFSA CEF Panel, 2009).
TDI	0.03 mg/kg bw/day (EFSA CEF Panel, 2009). DNEL: 0.05 mg/kg bw/day (ECHA, 2020) . TDI-value forms the basis for calculation.
Calculated highest acceptable concentration in baby body lotion*	13 mg/kg (results in a MoS value of 10)
Calculated highest acceptable concentration in shampoo*	9799 mg/kg (results in a MoS value of 10)

*Based on an allocation of 10 % TDI for cosmetic products as well as parameters indicated above and exposure calculated as indicated in section 5.3, the highest acceptable concentration can be calculated.

5.4.4 2,4-Di-tert-butylphenol

TABLE 27 Assessment and data applied in the safety assessment of 2,4-Di-tert-butylphenol.

CAS	96-76-4
Harmonized classification (health) and occurrence on REACH lists	Registry self-classify the substance as skin irritant (Skin Irrit2), i.e., no harmonized classification.

	REACH: under assessment as endocrine disrupting.
Cosmetics regulation	Not mentioned, i.e., in principle allowed.
SML in FCM regulation	None. Substance is not allowed as additive.
Skin permeability	No data found, which is why 1 is used by default.
NOAEL	20 mg/kg bw/day Critical effects on liver and kidneys (Miljøstyrelsen, 2007).
TDI	0.007 mg/kg bw/day (Miljøstyrelsen, 2007).
Calculated highest acceptable concentration in baby body lotion*	2 mg/kg (results in a MoS of 11 and 2.1 mg/kg gives MoS of 10)
Calculated highest acceptable concentration in shampoo*	150 mg/kg (results in a MoS value of 10)

* Based on an allocation of 10 % TDI for cosmetic products as well as parameters indicated above and exposure calculated as indicated in section 5.3, the highest acceptable concentration can be calculated.

5.4.5 2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT)

TABLE 28 Assessment and data applied in the safety assessment of BHT.

CAS	**128-37-0**
Harmonized classification (health) and occurrence on REACH lists	Under assessment as endocrine disrupting.
Cosmetics regulation	Not mentioned, i.e., in principle allowed.
SML in FCM regulation	3 mg/kg food or product simulant.
Skin permeability	0.134 (ECHA, 2020)
NOAEL	25 mg/kg bw/day Critical effects on liver and thyroid. (ECHA, 2020) (EFSA ANS Panel, 2012)
TDI	DNEL (general population – dermal route): 0.25 mg/kg bw/day (ECHA, 2020) (EFSA ANS Panel, 2012)
Calculated highest acceptable concentration in baby body lotion*	550 mg/kg (results in a MoS value of 10)
Calculated highest acceptable concentration in shampoo*	36560 mg/kg (results in a MoS value of 10)

*Based on an allocation of 10 % TDI for cosmetic products as well as parameters indicated above and exposure calculated as indicated in section 5.3, the highest acceptable concentration can be calculated.

5.4.6 Tris-(2,4-di-t-butylphenyl)phosphite

TABLE 29 Assessment and data applied in the safety assessment of tris-(2,4-di-t-butylphenyl)phosphite.

CAS	**31570-04-4**
Harmonized classification (health) and occurrence on REACH lists	None. Substance is registered.
Cosmetics regulation	Not mentioned, i.e. in principle allowed.
SML in FCM regulation	None. Substance is allowed as additive in FCM Regulation.
Skin permeability	No data found, which is why 1 is used by default.
NOAEL	58 mg/kg bw/day (ECHA)
TDI	0,6 mg/kg bw/day (ECHA)

Calculated highest acceptable concentration in baby body lotion*	190 mg/kg (results in a MoS value of 10)
Calculated highest acceptable concentration in shampoo*	11757 mg/kg (results in a MoS value of 10)

*Based on an allocation of 10 % TDI for cosmetic products as well as parameters indicated above and exposure calculated as indicated in section 5.3, the highest acceptable concentration can be calculated.

5.4.7 Additional comments on other substances

Alkanes have been identified in the product simulant through the GC/MS screenings. These can be included in the Cosmetic Regulation, Annex II (list of prohibited substances in chemical products). For instance, the following has been indicated as a prohibited substance/group of substances: Reference number 881: "*Alkanes, C1 2-26, branched and linear, except if the full refining history is known and it can be shown that the substance from which it is produced is not a carcinogen".* In cases with PCR plastic, alkanes are likely to originate from the degradation of polyolefins and their additives. Thus, they are not necessarily considered as carcinogenic, but must assessed specifically. In other cases, alkanes are mentioned in the form of various mineral oil fractions, where the criteria for their inclusion on the list of prohibited substances is that they must contain more than 0.1 weight percentage of butadiene. Butadiene has not been included in the analyses of PCT plastic samples in this project.

Fragrant substances, for example, limonene and alpha-hexylcinnamaldehyde, are substances which cause contact allergy to many consumers, and thus must be declared in concentrations above 0.001 % in leave-on products and 0.01 % in rinse-off products. If fragrant substances are technically unavoidable, it should be considered if the odor makes the packaging unsuitable for products that are labelled "perfume-free".

Octocrylene has been found in three samples in a concentration of up to 23 mg/kg. Octocrylene has a low SML value of 0.05 mg/kg, which indicates that it is more toxic than many other substances and should be assessed in relation to whether the concentration is safe for the respective application.

Remaining substances detected during analysis: Substances selected for the above safety assessment have been chosen in a detailed review of the analyses results. Hence, many substances have been left behind, which should be included if a complete safety assessment of the indicated PCR material is to be performed.

5.5 Calculations for selected PCR plastic samples and substances

The following section provides a summary and a comparison of the detected maximum acceptable concentrations for six selected substances/groups of substances in seven analyzed PCR plastic samples for baby body lotion and shampoo, respectively (described in section 5.3). The exposure scenario for baby body lotion is used as an example for one of the most sensitive applications (worst case), while shampoo for adults is used as a contrast, where the exposure is significantly lower (least sensitive). In addition to the maximum acceptable concentrations, margins of safety (MoS) for the six selected substances/groups of substances of three of the analyzed PCR plastic samples have been calculated based on the actual measured concentrations. These three PCR plastic samples have been selected as examples on PCR materials, which based on the analyses results, had a low, medium, or high level of migrated substances. An overview of the data used in MoS calculations for these three PCR plastic samples can be found in Appendix 7.

The maximum acceptable concentrations are, as mentioned, based on a MoS value of 10 in relation to TDI and not NOAEL, as TDI implicitly includes an assessment of NOAEL in the form

of uncertainty factors determined according to the quality of data and studies. This can establish an overall requirement for a MoS of at least 10, as 10% of TDI is generally allocated to cosmetics, but there can also be other sources of exposure to these substances than cosmetics. For example, it is known that degradation products of antioxidants such as 2,4-di-tert-butylphenol and BHT are released from drinking water installations and FCM plastic, and that phthalates are released from consumer products from soft PVC such as vinyl flooring, where the consumer is highly exposed via indoor climate air (Andersen, et al., 2012).

The maximum acceptable concentrations have been compared to the actual measured concentrations shown in TABLE 30, where values shown in red indicate values exceeding the maximum acceptable concentration. Both the maximum acceptable concentration of tris-(2,4-di-t-butylphenyl)phosphite and the maximum acceptable concentration of phthalates DEHP and DBP have been exceeded in sample no. 3.5 according to the scenario for baby body lotion. In case of the same scenario, the maximum acceptable concentration of 2,4-di-tert-butylphenol has been exceeded in all samples, except sample no. 1.1, which means that these PCR materials cannot be directly used as packaging for baby body lotion.

Corresponding conclusions are drawn from TABLE 31, which shows the calculated MoS values. Here, it can be seen that the MoS value for 2,4-di-tert-butylphenol is below 10 in sample no. 5.4 and no. 5.3 for baby body lotion, while sample no. 1.1 for Tris-(2,4-di-t-butylphenyl)phosphite has a MoS value of 17 for baby body lotion, which means that it will not require much variation/uncertainty before it can fall below the limit of 10. All substances in the exposure scenario with “shampoo” have MoS > 10 and thus are not problematic. In general, the MoS values are higher for shampoo than for baby body lotion, because shampoo, among others, is a rinse-off product, while body lotion remains on the skin.

The measured concentrations of the assessed substances are detected in ppm in the product simulant after a 3-day migration at 60 ºC. This means that the concentration indicates the amount of the substance, which over time can migrate from the granules into the cosmetic product. The measurements have been made with a surface/volume ratio of 1:1, which, for example, corresponds to a cream in small packaging for children, travel packaging and packaging sizes used at the hotel industry. Since the packaging material may be in contact with the cosmetic product for several years, it is realistic to assume that the substance in the packaging may over time diffuse into the cosmetic product until a balance is reached.

This safety assessment applies a surface/volume ratio of 1:1, which means that a relative dilution can be expected if larger containers are used (i.e., large amount of product in relation to packaging), and/or only a small proportion of PCR plastic used in the final plastic packaging. Thus, if the packaging is made with a large container volume and/or small material thickness, a lower amount of migrated substance into the packaged cosmetic product can be expected, thus achieving a safer application.

Uncertainties of analyses results vary from “unknown”, above 15 % to 50 %, which can be seen in TABLE 32. This is important for the assessment of the concentration of those substances that are just above the acceptable limit, for example, 2,4-di-tert-butylphenol. In case of other substances/product combinations, the analyses uncertainty in current cases does not cause any changes to this initial safety assessment. However, it must be noted that substance concentrations measured with screening methods with unknown uncertainty should be quantified through substance-specific analyses prior a final safety assessment. Furthermore, some estimates and “uncertainties” are also associated with some of the data applied in the safety calculations.

TABLE 30 Comparison of analyses results and the maximum acceptable concentrations in baby body lotion and shampoo, respectively. Numbers in red indicate values exceeding the maximum acceptable concentration in baby body lotion. No measured concentrations exceed the maximum acceptable concentration in shampoo.

Name of substance	CAS No.	Max. acceptable conc. (mg/kg) Baby body lotion Shampoo	Measured conc. (mg/kg) Sample 1.1	Measured conc. (mg/kg) Sample 2.1	Measured conc. (mg/kg) Sample 3.3	Measured conc. (mg/kg) Sample 3.5	Measured conc. (mg/kg) Sample 4.2	Measured conc. (mg/kg) Sample 5.3	Measured conc. (mg/kg) Sample 5.4
Benzophenone	119-61-9	**13** **9799 (0.9%)**	1.2	0.59	2.2	0.25	-	-	0.58
Dibutyl phthalate (DBP)	84-74-2	**20** **1315 (0.1%)**	0.098	0.14	7.8	0.54	0.24	4.5	1.8
Diethylhexyl phthalate (DEHP)	117-81-7	**295** **19595**	5.6	-	42	220	44	10	-
Sum of DEHP, DBP (x5)	-	**148** **9798**	6.1	-	81	**223**	45	33	-
Tris-(2,4-di-t-butylphenyl) phosphite	31570-04-4	**190** **11757**	110	140	-	22	**1000**	-	3.8
2,4-Di-tert-butylphenol	96-76-4	**2** **150**	-	**2.2**	**4.1**	**2.0**	**4.5**	**6.5**	**4.6**
2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	**550** **36560**	0.33	0.38	1,7	0.67	-	5.9	2.4
Other substances (triviality limit)	-	**0.0008** **0.049**							

TABLE 31 Comparison of analyses results with the calculated MoS values and the maximum acceptable concentrations for baby body lotion and shampoo, respectively. Numbers in red indicate values exceeding MoS values for baby body lotion.

Name of substance	CAS No.	Max. acceptable conc. (mg/kg) Baby body lotion Shampoo	Measured conc. (mg/kg)	MoS= TDI/SED Baby body lotion Shampoo	Measured conc. (mg/kg)	MoS= TDI/SED Baby body lotion Shampoo	Measured conc. (mg/kg)	MoS= TDI/SED Baby body lotion Shampoo
			Sample 1.1		Sample 5.3		Sample 5.4	
Benzophenone	119-61-9	**13** **9799 (0.9%)**	1.2	110 7349	-	-	0.58	228 15204
Dibutyl phthalate (DBP)	84-74-2	**20** **1315 (0.1%)**	0.098	2113 140674	4.5	46 3064	1.8	115 7659
Diethylhexyl phthalate (DEHP)	117-81-7	**295** **19595**	5.6	552 36743	10	309 20576	-	-
Sum of DEHP, DBP (x5)	-	**148** **9798**	6.09	254 16893	32.5	48 3166	-	-
Tris-(2,4-di-t-butylphenyl) phosphite	31570-04-4	**190** **11757**	110	17 1122	-	- -	3,8	488 32489
2,4-Di-tert-butylphenol	96-76-4	**2** **150**	-	- -	**6.5**	3 222	**4.6**	5 313
2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	**550** **36560**	0.33	17476 1163282	5.9	977 65065	2.4	2403 159951
Other substances (triviality limit)	-	**0.0008** **0.049**						

TABLE 32 Analysis methods and uncertainties for the assessed substances.

Substance (group)	Applied analysis method	Product simulant	Uncertainty	Impact on safety assessment
Aluminum	ICP/MS screening	Acetic acid	Unknown	Unknown
Benzophenone	LC/MS multitarget analysis	95 % ethanol	50 % RSD	Even with analysis uncertainty, the concentration is within acceptable limit.
Dibutyl phthalate (DBP)	LC/MS multitarget analysis	95 % ethanol	50 % RSD	In this case, this uncertainty does not cause any changes to the conclusion.
Diethylhexyl phthalate (DEHP)	GC/MS screening	Isooctane	Unknown	Unknown
Tris-(2,4-di-t-butylphenyl) phosphite	GC/MS screening	Isooctane	Unknown	Unknown
2,4-Di-tert-butylphenol	GC/MS (PE-phenols)	95 % ethanol	15 % RSD	Uncertainty on the analysis cause an uncertainty regarding the exceeding of the acceptable level in two of the samples. The others are still clearly above acceptable limits for baby body lotion. For shampoo, all actual concentrations are acceptable, even with this uncertainty.
2,6-Bis(1,1-dimethyl)-4-methylphenol (BHT)	GC/MS (PE-phenols)	95 % ethanol	15 % RSD	Even with analysis uncertainty, the concentration is within acceptable limit.

5.6 Guide for safety assessment of PCR plastic for packaging of cosmetic products

Cosmetics Europe's "*Advisory document on information exchange on cosmetic packaging materials along the value chain in the context of the EU cosmetics regulation EC 1223/2009"* (Cosmetics Europe, 2019) states the proposed principles of industry association on which type of information on ingredient substances is reasonable to request in packaging for being able to safety assess the specific use of the packaging. It proposes that, as a starting point, information corresponding to the declaration of conformity for food contact materials is requested. In addition, information should be requested on substances subject to prohibitions or restrictions according to the Cosmetic Regulation, in addition to substances that are classified as skin sensitizing. As stated in this report, this approach is not sufficient for PCR plastics.

When calculating exposure of different substances, the standard exposure scenarios or Appendix 7 should be applied for the different cosmetic types such as body lotion and shampoo, as indicated in *'Notes of Guidance'* (SCCS, 2018).

5.6.1 How to ensure that everything is included?

The results of this project show that one easily end up with long lists of substances which must be investigated in relation to whether the concentration is too high for the specific use of packaging. One should typically look for data on substances at:

- echa.europa.eu/da/information-on-chemicals: Information on potential CMR-classification, suspected endocrine disrupting effects, occurrence on the candidate, restriction and authorization list as well as the registrant's own assessment of substances.
- Annex II to the Cosmetic Regulation: List of substances which are prohibited in cosmetic products.
- Annex III to the Cosmetic Regulation: List of substances which cosmetic products must not contain except subject to the fixed limitations.
- Annex V to the Cosmetic Regulation: List of preservatives allowed in cosmetic products.
- Annex VI to the Cosmetic Regulation: List of UV filters allowed in cosmetic products.
- Annex I to the FCM Regulation: List of monomers, additives, etc. allowed in plastic food contact materials. Also contains information on specific migration limit values for foods. Often, you will be able to find background documents in the form of EFSA or other scientific committee assessment of substances.

A systematic review of the analyzed substances in relation to their presence on the above lists has not been possible to perform within the framework of this project. The numerical data set is too large to be able to review without employing digital tools.

In most cases, the CAS number is used for reference, but there are also some exceptions, where group designations without CAS numbers have been used in the lists. A possible digital search tool should be able to take this feature into account.

Even if no classification of the substance is available, or the substance does not occur on any of the above-mentioned lists, it should nevertheless be investigated whether any toxicological effects are described in scientific literature. This is because only those substances are included on the lists that are relevant to their specific use, and that lists are not exhaustive for all substances that can be present in plastic materials. In such cases, it must be assessed whether there is a reason to exclude those PCR plastic materials which include the substance.

Some worst-case calculations

For substances with no TDI or ADI values and where the chronic toxicity has not been thoroughly investigated in long-term studies (e.g., NOAEL value for systemic effects after oral administration in repeated dose-response-study), a worst-case scenario should be applied. In a

worst-case scenario, the lowest exposure which can cause a toxicological effect (TTC) according to EFSA (EFSA, 2019) is applied. The TTC value is used to replace TDI for substances with very limited information. TTC values for substances with a potential of being DNA reactive mutagens and/or carcinogens, or which do not have data to exclude these effects, are set to be the TTC value (TDI) of 0.0025 µg/kg bw/day (EFSA, 2019) (SCCS, 2018).

The TDI value covers a person's total exposure from all sources of a specific substance. Since one can be exposed to the same substance from several sources, for example from food contact materials, consumer products and drinking water installations, 10% of TDI value is allocated to cosmetics. This means that the MoS value must be 10 or above for a concentration of a substance to be safe.

If it is assumed hereof that the substance can easily be absorbed through the skin (P = 1, i.e., 100% of substance is absorbed through skin) and TTC of 0.0000025 mg/kg bw/day (2.5×10^{-6}), the maximum allowed concentrations can be calculated for packaging for baby body lotion and shampoo, respectively. In case of baby body lotion, it means that the measured concentration must not exceed 0.0008 mg/kg, i.e., 0.8 µg/kg, and for shampoo max. 0.049 mg/kg, i.e. 49 µg/kg (as it ensures a MoS value of 10 and above). Thus, the value of 0.8 µg/kg could be stated as the 'triviality limit' in cosmetic products for skin contact.

However, the calculated triviality limits of 0.8 µg/kg for baby body lotion and 49 µg/kg for shampoo are so low that they are below the usual detection limits in the typical analyses that can be performed.

Furthermore, the following examples (for baby body lotion) on substances with an available TDI value can be used as a starting point:

- For substances, which are easily absorbed through skin (P = 1), and a TDI value of 1 mg/kg bw/day, the measured concentration can be maximum 300 mg/kg (as it results in a MoS value of 10).
- For substances, which are easily absorbed through skin (P = 1), and a TDI value of 10 mg/kg bw/day, the measured concentration can be maximum 3000 mg/kg (as it results in a MoS value of 10).
- For substances, which are only partially absorbed through skin (P=0.1), and a TDI value of 10 mg/kg bw/day, the measured concentration can be max. 30000 mg/kg (as it results in a MoS value of 10).

5.7 Conclusion on safety assessment

In general, the safety assessment of the selected substances/groups of substances in the examined PCR plastic materials shows that plastic materials may be used as packaging for some cosmetic products, even in cases, where the migration of the substance exceeds the accepted values for plastic for food contact. The usage of PCR plastic for packaging of shampoo is mainly safer than for baby body lotion, as shampoo is rinsed off after application, and because the exposure typically occurs to a relatively larger body weight compared to skin surface area.

According to calculations for substances in this project, it appears that in many cases 2,4-di-tert-butylphenol exceeds the acceptable level. Similarly, both phthalates and tris-(2,4-di-t-butylphenyl) phosphite in some cases exceed the acceptable level as well. Thus, the tested PCR plastic samples cannot be used for packaging of baby body lotion.

An infinite number of substances can potentially migrate from PCR plastic, as the plastic materials can naturally originate from many sources and have had many different applications during the lifetime at the consumer. The analyses detected numerous more substances than what was possible to safety assess in this project due to limited resources, and thus it cannot be ruled out that other problematic substances that were not detected may be present. Based on the list of detected substances, it is possible to select substances for safety assessment according to the screening of substance TDI and skin permeability. If the PCR plastic material is to be used in baby body lotion, the following criteria can be derived from calculations made in the project:

- For substances, which are easily absorbed through skin (P = 1), and a TDI value of 1 mg/kg bw/day, the measured concentration can be maximum 300 mg/kg (as it results in a MoS value of 10).
- For substances, which are easily absorbed through skin (P = 1), and a TDI value of 10 mg/kg bw/day, the measured concentration can be maximum 3000 mg/kg (as it results in a MoS value of 10).
- For substances, which are only partially absorbed through skin (P=0.1), and a TDI value of 10 mg/kg bw/day, the measured concentration can be max. 30000 mg/kg (as it results in a MoS value of 10).

A full safety assessment of a specific PCR plastic material must include all problematic substances detected in the chemical analyses, where these are assessed according to whether the measured concentrations are safe for the specific use of the packaging (which in practice would be an extensive task). Furthermore, a full safety assessment must also consider, whether the applied analysis methods are able to detect all relevant substances in the relevant concentrations. For instance, some substances would only migrate when using more polar simulants, and also some substances would not be detected or quantified due to interference in the selected analysis method.

Since all substances could not be included in a safety assessment, a general “triviality limit” for migration of substances was calculated. The triviality limit is 0.8 µg/kg product for migrated substances from plastic materials, which are used for packaging of cosmetic products for skin contact (leave-on). If PCR plastic material must be used for packaging of hair shampoo, the triviality limit can thus be increased to 49 µg/kg shampoo. The triviality limit has been calculated based on available equivalent to the most hazardous chemical substances, even though it is considered unlikely that exactly these are present in PCR plastic. However, the calculated triviality limits are so low that they are below the usual detection limits in the typical analyses that can be performed. Thus, their practical use is limited.

6. Discussion

This chapter describes first the dialog with relevant stakeholders from the industry concerning the results of the project and provides a discussion of the uncertainties and shortcomings as well as the knowledge lacking for being able to use PCR plastic of polyolefins in cosmetic packaging. This has been identified partly by the project group during this project, and partly through a dialog with the relevant stakeholders from the industry.

6.1 Dialog with relevant stakeholders from the industry

This project was initiated from a demand for greater knowledge in the field requested by, among others, manufacturers of cosmetic products, packaging manufacturers and plastic reprocessing plants. These stakeholders have contributed to the project by submitting documentation and PCR plastic samples for analyses and safety assessment (reviewed in chapter 2). The preliminary results of this project were presented at an online workshop with these stakeholders, which involved a discussion of the results and opportunities for using PCR plastic in cosmetic packaging.

At the workshop, it was clear that the industry desires clear guidelines with a well-described procedure for what is to be tested, documented, and fulfilled if PCR plastic materials were to be used for packaging of cosmetics and personal care products.

The industry stakeholders expressed a general concern about whether it was realistic to be able to use PCR plastic for cosmetic packaging if analyses and documentation are required for all batches. The concern was also related to the fact that toxic substances could be present in the plastic after migration at the consumers and in practice it is impossible to test all batches for all chemical substances.

In this case, the only solution for access to reliable, controlled, and safe PCR plastic materials would be the establishment of closed collection loops/take-back-systems for manufacturer's own packaging. Only this way, the manufacturer would be able to document the chemical content in virgin plastic and chemical substances in PCR plastic materials. However, it must be mentioned that also in this case the consumers may have contaminated the plastic with undesirable chemical substances.

As an alternative to having to analyze all chemical substances, the project group added that in many cases a closer analysis and control of PCR plastic material source, i.e., collection, sorting and reprocessing, may help to identify the most common problematic substances. In the long run, it would be possible to develop a targeted analyses program, which can detect the most undesirable substances.

It may also be possible to develop a reprocessing procedure for the removal or reduction of undesirable substances based on knowledge on which substances should potentially be removed. Then, it should be documented that the procedure removes the selected substances. Exactly this procedure is used for recycling of PCR plastic materials of PET, for, e.g., packaging. Here, the reprocessing procedure must be approved for its ability to purify PET with a specific effectiveness for a range of chemical model substances of varying boiling points and polar/nonpolar properties. After this, the process is expected to be able to reprocess received post-consumer PET to rPET of food quality.

Such approval procedures typically take place via the so-called challenge-tests (EFSA, 2011). It must be noted that the responsibility for the chemical safety remains with those who bring the pre-packaged product to market.

Finally, the industry stakeholders expressed a wish to be able to continue the work and ensure continuous involvement of the industry in the Danish Environmental Protection Agency's work in this field. It was specifically proposed to establish a panel of stakeholders to follow up on this study and possibly facilitate new initiates in this field.

6.2 Uncertainties and shortcomings of this study

This project provides a limited study on selected samples of PCR plastic materials from Danish stakeholders' sources from the available batches of these. A limited analysis program was carried out, where seven samples were analyzed at screening level, and for four of these samples a range of selected specific substances was quantified with more detailed analyses. According to a review of the substances detected in the chemical analyses with an assessment of which substances are directly considered as problematic to health, six substances/groups of substances of the identified substances in the seven analyzed samples were selected for safety assessment.

The results are merely a snapshot of the main part of the content of chemical substances, but it cannot be expected to clarify the general content of all possible chemical contaminants. For a small number of substances, the importance of the chemical safety has been risk assessed regarding the use of these materials in packaging of cosmetic products. Hence, the results of this study are not sufficient to be able to guarantee that PCR plastic material from a specific reprocessed batch of PCR plastic is safe to use, and here the expected variation from batch to batch should be mentioned, which has not been investigated in this project.

The analysis program was established based on the number of samples and analyses possible within the financial and time framework of this project. In case of an in-depth study, it would have been preferable to perform the broad, semi-quantitative screening analyses first and thereafter select specific substances or groups of substances for quantitative analysis. Likewise, the list of selected substances (presented in section 3.3), for which it is relevant to analyze PCR plastic materials, could have been more comprehensive in terms of chemical legal requirements and safety concerns, if the project framework had allowed it.

The selection of product simulants is a compromise between expected properties of personal care products, analytic technical limitations, and the scope/availability of analyses opportunities within the framework of this project. As mentioned, migration liquids have been chosen primarily to be able to simulate fatty products, which are not rinsed off (leave-on) in a worst-case situation, that is, migration liquids that are expected to extract as many chemical substances from PE or PP plastic matric as possible. These product simulants are expected to extract more chemical substances from plastic than many cosmetic products, which are not purified, as many of these products consist of more polar emulsions compared to nonpolar fat or oil-based products. However, it cannot be ruled out that specific, more polar chemical components would migrate into plastic to a greater extent if a more polar product simulant had been used. Finally, in some cases analytic technical limitations apply, for example, in the analysis of PAA, which cannot be performed on non-polar migration liquids, which is why a 3% acetic acid is used instead, i.e., a polar migration liquid that simulates a water-based product. It cannot be ruled out that a greater amount of PAA could have been detected in the analysis if it had been performed after migration to, e.g., isooctane.

The project has not systematically studied the effects of different product simulants, although this is expected to have a great impact on the results of the chemical analyses and thus the

following safety assessments. In the project, the safety assessments have been performed by taking product simulants into consideration. Therefore, scenarios were created for baby body lotion (assumed fat-based) and shampoo (assumed water-based), where the results for both polar and non-polar migrations have been used. A more ideal safety assessment would base the assessment of substances in a fatty product on the analyses performed on a non-polar migration liquid, and substances in water-based products on analyses performed on polar migration liquid, but since many cosmetic products are emulsions of different polar and non-polar components, the discussion about the most suitable product simulants is not straightforward after all. Additionally, there may be uncertainty about how true a fat simulant can be to creams that are emulsions with a varying degree of fat content.

Furthermore, the safety assessments include the ratio between the amount of sample granules of PCR plastic and the migration liquid corresponding to the ratio between the mass of plastic packaging and the amount of the cosmetic or personal care product. For the safety assessment in this project, this ratio is assumed to be approx. 1:1, which again can be considered as a worst-case scenario. When an amount of a product is equal to the amount of packaging, in practice it corresponds to, for example, a small travel-size packaging of body lotion. For standard packaging of personal care products, there is often more product than packaging if measured on mass.

In general, it is expected that the concentration of possible chemical substances migrated from the packaging will usually be smaller than the one found in this project, as several worst-case scenarios have been taken into consideration. However, it must be noted that for the analysis an initial selection of PCR plastic materials was made, which were expected to be accepted as packaging materials based on the performed safety assessment.

To sum up, it can be concluded that a more detailed (and possibly improved) safety assessment could be performed if the following is included:

- Systematic study of the variation in materials from different waste sources, recycling processes, batches, and sampling materials.
- Use of product simulants, which can be compared to the specific products for which the material is intended to be used as packaging (or at least an increased knowledge on the effect of product simulants on the analyses results).
- Use of actual packaging/product-ratio both for safety assessment and during the actual migration (for example, by performing a migration study on a pre-molded plastic packaging).
- A more detailed study in connection with selection, analysis, and assessment of the correct chemical substances (for example, by running several broader screenings initially and then focusing on the substance-specific analyses later).
- More toxicological data, e.g., on absorption of chemical substances through skin.
- Safety assessment of many more of the identified components and different use scenarios.

6.3 Recommendations for further studies

The work with analyses and safety assessment of PCR materials clearly indicates that this project is merely the first step towards a safe application of PCR plastic materials of PE and PP in cosmetic and personal care products. The results are positive in terms of being able to use PCR plastic materials to produce, for example, shampoo bottles of PCR-PE-plastic, but it has also been obvious that it is challenging to develop a clear procedure for the manufacturers to document a safe use of possible PCR plastic materials in the future.

First, it is relevant to compare the existing results from migration studies and chemical analyses to similar analysis on virgin packaging materials of PE and PP. Since many of the analyzed substances are carbon chains, it is possible that most of the identified components originate from the original plastic materials (or their degradation) and is not contamination from use phase. This could indicate that the identified chemical substances in PCR materials may not be that different from those in virgin polyolefins.

In addition to performing several detailed, substance-specific chemical analyses, there is also the potential for initiatives which can eliminate or at least reduce some of the mentioned uncertainties and shortcomings mentioned in section 6.2. This could be done, for example, by analyzing several of the collected PCR plastic materials, collecting more analysis samples from each material, closer reviewing the screening results to be able to select several substances for quantitative analyses and perform safety assessments of many more substances based on the already available results.

Furthermore, it would be useful to develop a digital tool that could automatically compare lists of identified chemical substances from screening analyses to several different lists of regulated and hazardous substances. This way, the potential chemical “showstoppers”, which prevent the opportunity from using PCR plastic materials, could be identified quickly. This can be technically done by comparing CAS numbers, as these do not vary to the same degree as chemical names. In addition, it will be necessary to process those substances that are regulated in substance groups without a CAS number, and substances with several possible CAS numbers.

Also, it is concluded that very useful knowledge can be gained from a systematic study of the effect of different migration liquids/product simulants and their properties compared with actual cosmetic products, as discussed above. As demonstrated in Appendix 2, product simulants have also an important role in the color migration from plastic to product, which is an important consideration in relation to the use as cosmetic packaging irrespective of the fact whether color migration is due to problematic or entirely harmless substances.

In addition to color migration, the odor of the PCR plastic materials is also an important factor, as all received PCR plastic materials gave off odor, and most of the samples had a strong fragrance. A more detailed study and understanding of the chemistry behind the odor would allow the manufacturer to make the right quality requirements, while reprocessing plants could be able to adjust the processes for odor reduction.

Finally, the sources, samples and batches in this project were determined by with what the industry had chosen to contribute to this project, which is why future studies could advantageously include a systematic comparison of the material quality from different waste sources/origins and possibly from different types of recycling processes. This way, it could be possible to identify whether the specific substances are often seen in special waste flows, or whether the specific processes reduce the presence of special substances. Even though this project has analyzed samples from the entire world and from different processes, the data foundation has been too small to be able to identify possible trends. Batch variations from the

same source and process have not been studied yet, but such a study would provide a valuable knowledge on whether the chemistry in different batches varies as much as feared, when it comes to PCR plastic materials.

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Appendix 1: PCR plastic samples

The following figures are photos of the received PCR samples that are all in the form of extruded pellets. The square dimensions are 5x5 mm.

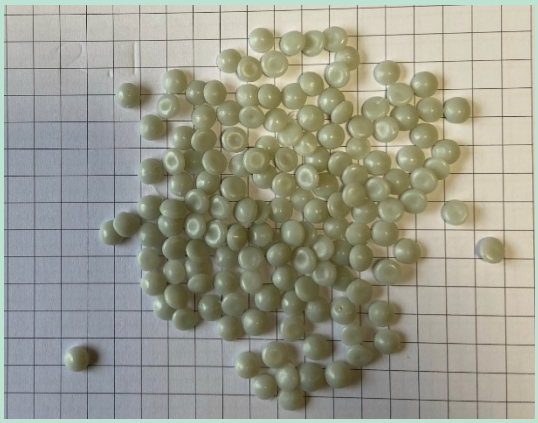

FIGURE 2. Sample 1.1.

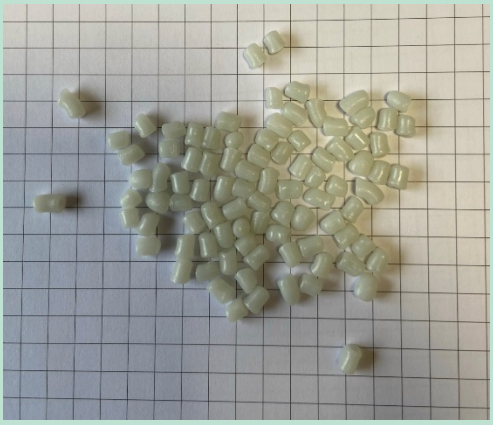

FIGURE 3. Sample 2.1.

FIGURE 4. Sample 3.1.

FIGURE 5. Sample 3.2.

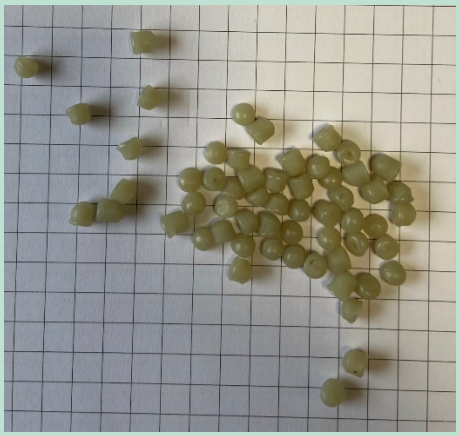

FIGURE 6. Sample 3.3.

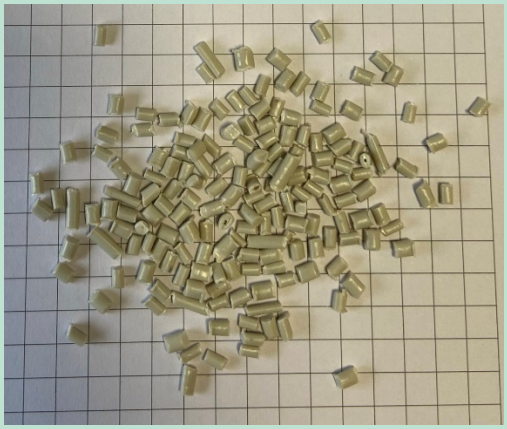

FIGURE 7. Sample 3.4.

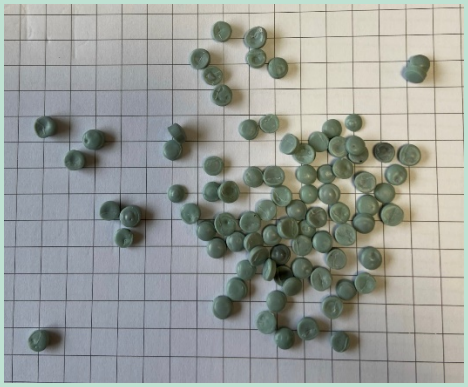

FIGURE 8. Sample 3.5.

FIGURE 9. Sample 3.6.

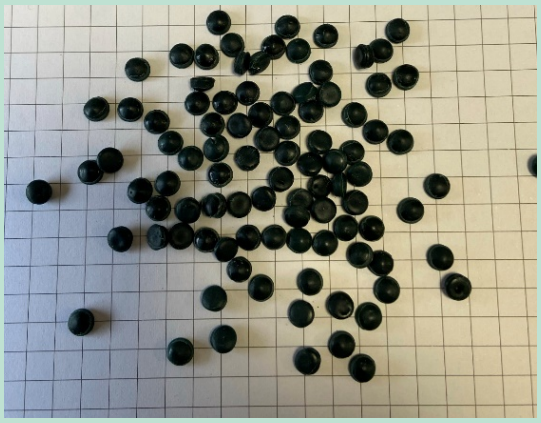

FIGURE 10. Sample 4.1.

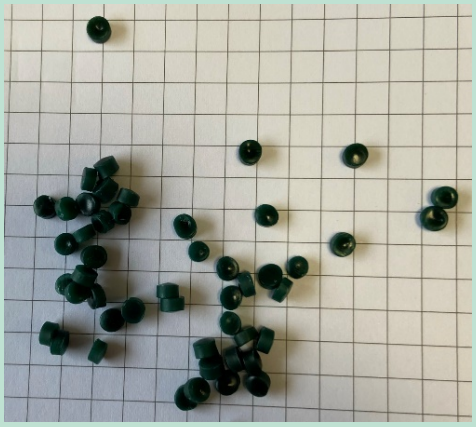

FIGURE 11. Sample 4.2.

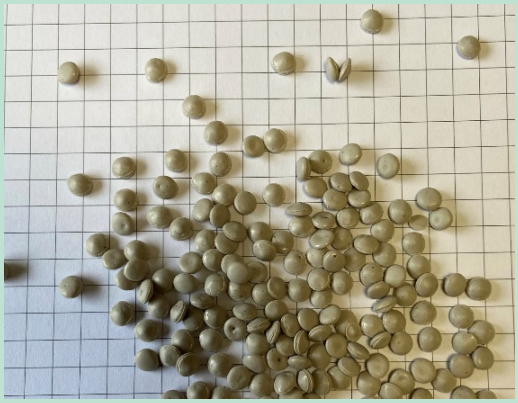

FIGURE 12. Sample 4.3.

FIGURE 13. Sample 4.4.

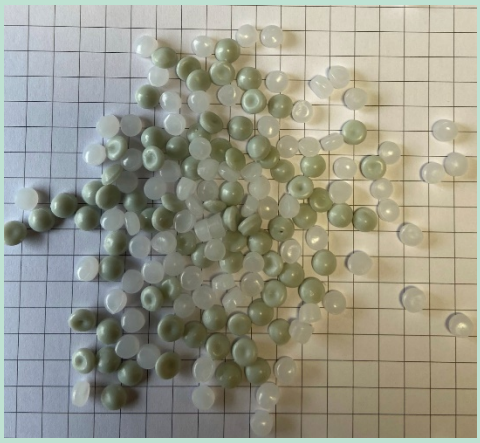

FIGURE 14. Sample 5.1.

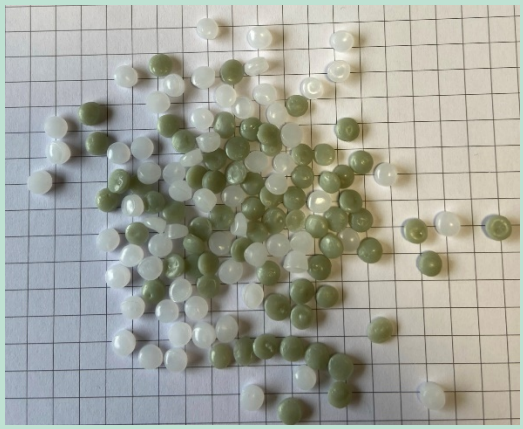

FIGURE 15. Sample 5.2.

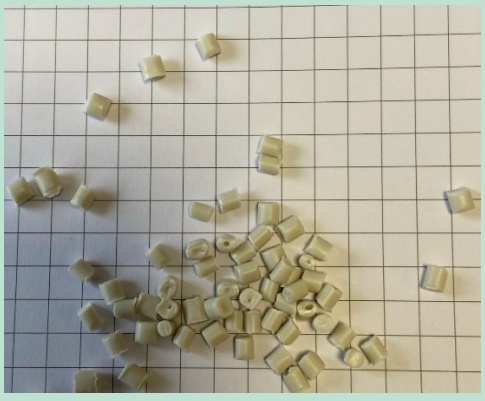

FIGURE 16. Sample 5.3.

FIGURE 17. Sample 5.4.

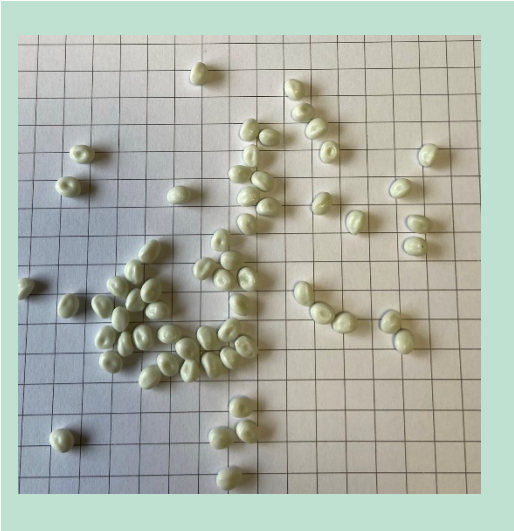

FIGURE 18. Sample 5.5.

Appendix 2: Migration

Appendix 2.1: Migration Conditions

TABLE 33 Migration conditions

Sample No.	Migration liquid/ Product simulant	Migration time [hours]	Temperature [°C]	Mass of resin [g]	Volume of migration liquid [mL]
1.1	3 % acetic acid	72	60	55.045	40
2.1	3 % acetic acid	72	60	55.120	40
3.5	3 % acetic acid	72	60	55.120	40
5.4	3 % acetic acid	72	60	55.240	40
1.1	95 % ethanol	72	60	35.050	30
2.1	95 % ethanol	72	60	35.080	30
3.3	95 % ethanol	72	60	35.120	30
3.5	95 % ethanol	72	60	35.050	30
4.2	95 % ethanol	72	60	35.120	30
5.3	95 % ethanol	72	60	35.020	30
5.4	95 % ethanol	72	60	35.050	30
1.1	Isooctane	72	60	35.370	30
2.1	Isooctane	72	60	35.050	30
3.3	Isooctane	72	60	35.400	30
3.5	Isooctane	72	60	35.090	30
4.2	Isooctane	72	60	35.050	30
5.3	Isooctane	72	60	35.260	30
5.4	Isooctane	72	60	35.150	30

Appendix 2.2: Images of migration to product simulant - isooctane

FIGURE 19. Image of samples immediately after migration to isooctane. From left to right, the samples are numbered 1.1, 2.1, 3.3, 3.5, 4.2, 5.3, and 5.4. It is visible that samples 4.2 and 5.3 have absorbed migratory liquid and are swollen.

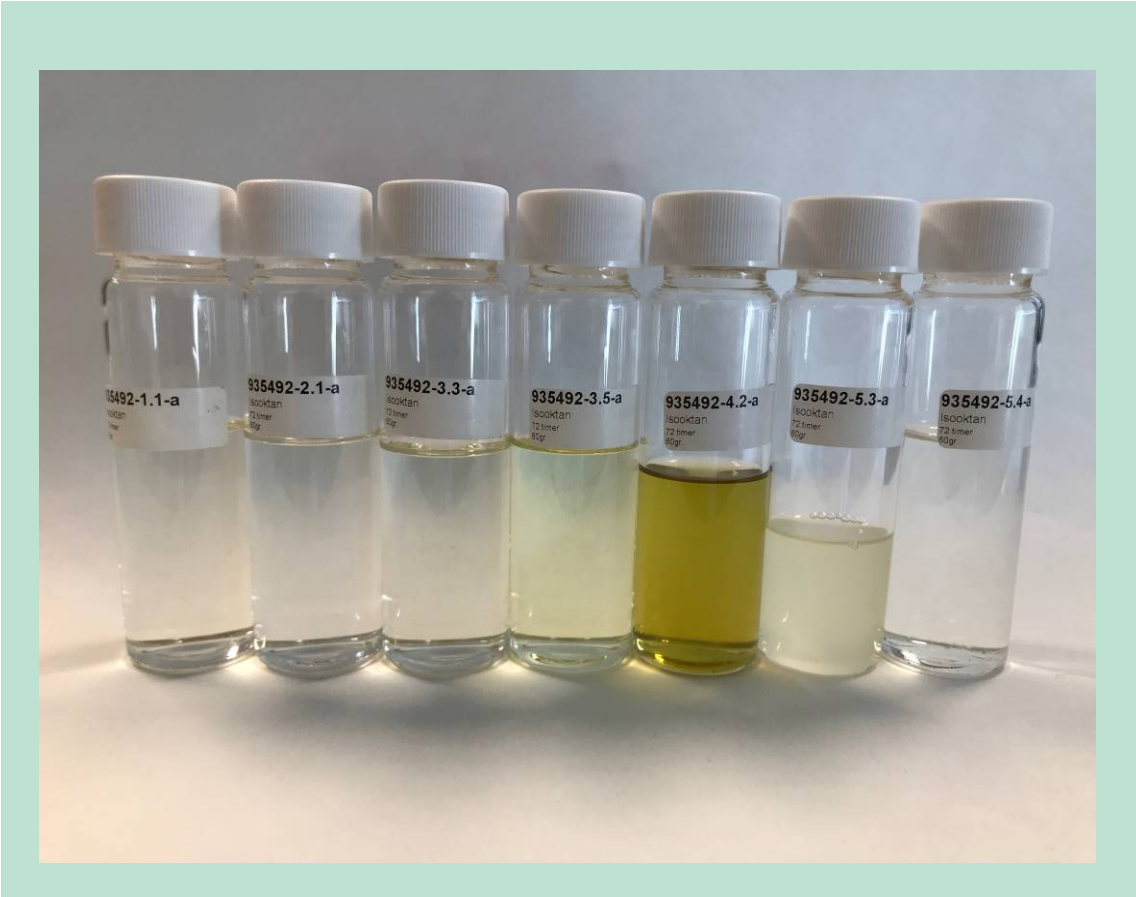

FIGURE 20. Image shows the migration liquid - isooctane extracted after migration. Some samples have acquired color from the migration. This is especially true for sample 4.2, which has acquired a lot of color. However, the color change was also observed in Sample 3.5 and Sample 5.3. The latter has also become cloudy, which may indicate that particles have been released into the migration liquid.

Appendix 2.3: Images of migration to product simulant - 95 % Ethanol

FIGURE 21 Image of samples immediately after migration to 95% ethanol. From left to right, the samples are numbered 1.1, 2.1, 3.3, 3.5, 4.2, 5.3, and 5.4. No swelling is observed.

FIGURE 22 Image shows the migration liquid - 95% ethanol extracted after migration. It is visible that some samples have acquired color from the migration. This applies to samples 3.5 and 4.2. No unclear phases are visible in sample 5.3 as observed when using isooctane.

Appendix 2.4: Images of migration to product simulant – 3% acetic acid

FIGURE 23 Image of samples immediately after migration to 3% acetic acid. No difference in the material is observed after migration. Note that the material floats on top, as the density of this migration liquid exceeds the density of the sample material.

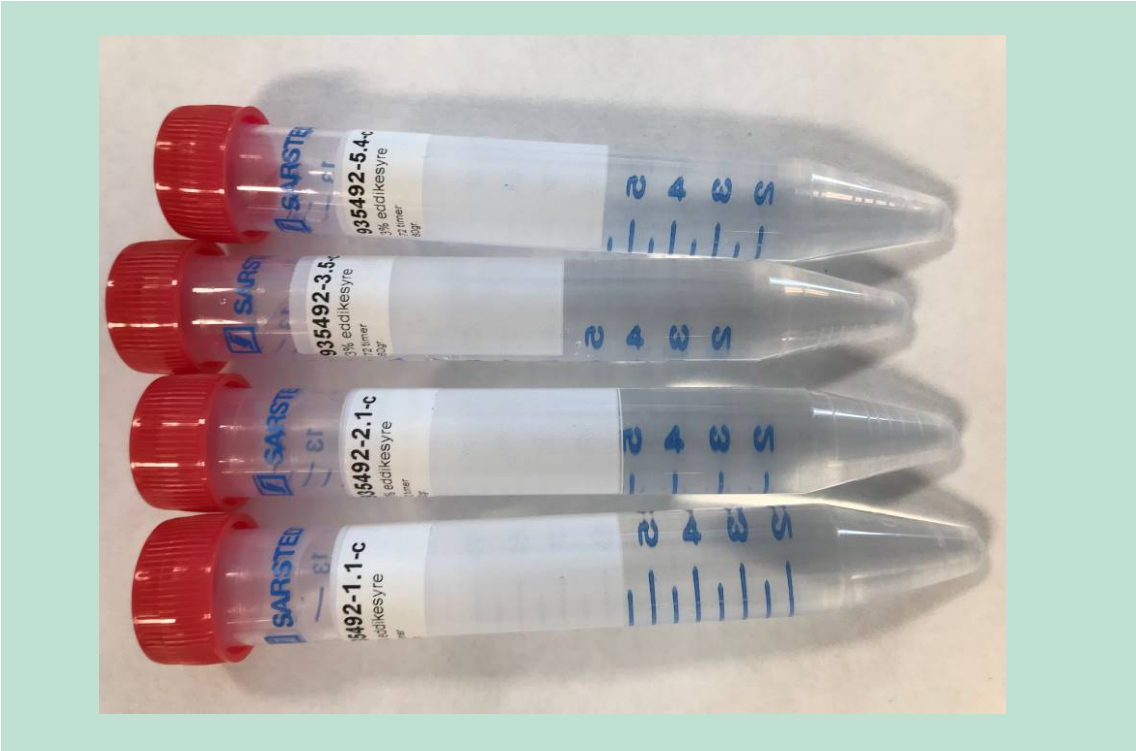

FIGURE 24 Image shows migration liquid (3% acetic acid) extracted after migration. Migration liquid is clear with no instances of unclear phases.

Appendix 3: Methodology

Appendix 3.1: GC/MS screening

A subset of the product simulant (isooctane) is extracted and diluted 1:1 with dichloromethane added internal standards. The extract was analyzed by gas chromatography with a mass selective detection (GC/MS). The identification of the measured components has been performed by comparing these with NIST MS library. The identification from the NIST library is considered only as guidance. For definitive positive identification, substance-specific analysis should be performed with reference substances. The content of the samples is calculated semi-quantitatively as naphthalene and has an unknown uncertainty.

Estimated detection limit: 3 mg/kg product simulant expressed as naphthalene equivalent.

The GC/MS screening has been performed semi-quantitatively, as it is not financially possible within the project to perform specific calibration of all substances present. By semi-quantitative analysis it is meant that no calibration is performed against the substance that is identified. Instead, it is calibrated to the response of the naphthalene, and therefore the detected amounts are referred to as naphthalene equivalents. Substances that are very similar to naphthalene will be determined with high precision (e.g., methylnaphthalene), while substances that are dissimilar will have a lower precision (e.g., citrate). GC/MS screening is a cheaper approach to getting broad information about a product rather than performing many specific analyses. Subsequently, specific analyses for problematic substances can be selected.

Appendix 3.2: LC/MS multitarget analysis

The product simulant (95% ethanol) is analyzed by internal assessment for the content of components presented using LC/MS. The analysis was performed by a subcontractor approved by the Danish Technological Institute.

Detection limit: 0.004 - 0.3 mg/kg product simulant, see also Appendix 5.
Dispersion: 50 % RSD

Appendix 3.3: ICP/MS screening

The samples have been analyzed according to the method of Danish Technological Institute: UA 263 ‘Semi-quantitative determination of elements by ICP/MS’.

The method is used for semi-quantitative determination of up to 67 elements from lithium to uranium. The method uses the principle of characteristic fingerprints and intensities of each element, which is calculated according to a curve based on a selection of quantified elements from traceable external standards. This gives a semi-quantitative determination of the individual elements in relation to each other and is associated with an unknown uncertainty.

A small amount of the product simulant (3% acetic acid) was acidified with nitric acid and prepared by microwave-induced heating. The resulting solution was diluted to 50 ml with Milli-Q water. The samples were analyzed for elemental content of ICP-MS with CCT in KED-mode and with He as collision gas. Ge, Rh and Re were used as internal standards.

Estimated detection limits are provided in Appendix 6.

Appendix 3.4: PAH analysis

A small amount of the product simulant (isooctane) was extracted and diluted 1:1 with dichloromethane with added internal standards. The extract was subsequently analyzed by gas chromatography with mass selective detection (GC/MS). The identification of the measured components is performed by comparing retention time and MS spectrum with external reference standards.

Detection limit: 0.2 mg/kg product simulant
Dispersion: 15 % RSD

Appendix 3.5: PAA analysis

The product simulant (3% acetic acid) was analyzed by internal analysis for content of the presented PAA using LC/MS. The analysis was performed by a subcontractor approved by the Danish Technological Institute.

Detection limit: 0.002 mg/kg product simulant
Dispersion: 20 %RSD

Appendix 3.6: PE-phenol analysis

A small amount of the product simulant (isooctane) was extracted and diluted 1:1 with dichloromethane with added internal standards. The extract was subsequently analyzed by gas chromatography with mass selective detection (GC/MS). The identification of the measured components was made by comparing retention time and MS spectrum with external reference standards.

Detection limit: 0.2 mg/kg product simulant
Dispersion: 15 % RSD

Appendix 3.7: PFAS-Analysis

A small amount of the sample material (resin) was extracted by Soxhlet extraction with methanol as solvent. The extract was analyzed by liquid chromatography using tandem mass spectrometry (LC/ MS/MS). The analysis was performed by a subcontractor approved by the Danish Technological Institute.

Detection limit: 0.005 mg/kg
Dispersion: 30 % RSD

Appendix 3.8: Total fluoride content

An amount of sample material was weighed and packed in nitrocellulose, which was placed in a bottle. The nitrocellulose was then ignited, and the combustion products passed through a alkalic solvent trap. Subsequently, the solvent trap was analyzed by ion chromatography with regards for the fluoride content. Reference method: EN 14582: 2016.

Detection limit: 20 mg/kg
Dispersion: 15 % RSD

Appendix 4: Complete GC/MS screenings

In the following, GC/MS screenings are presented. The screenings were performed and presented in English. The migration into isooctane was performed over a period of 3 days at 60 °C. Isooctane was then extracted and analyzed. Results are expressed as [mg] analyte per [kg] product simulant.

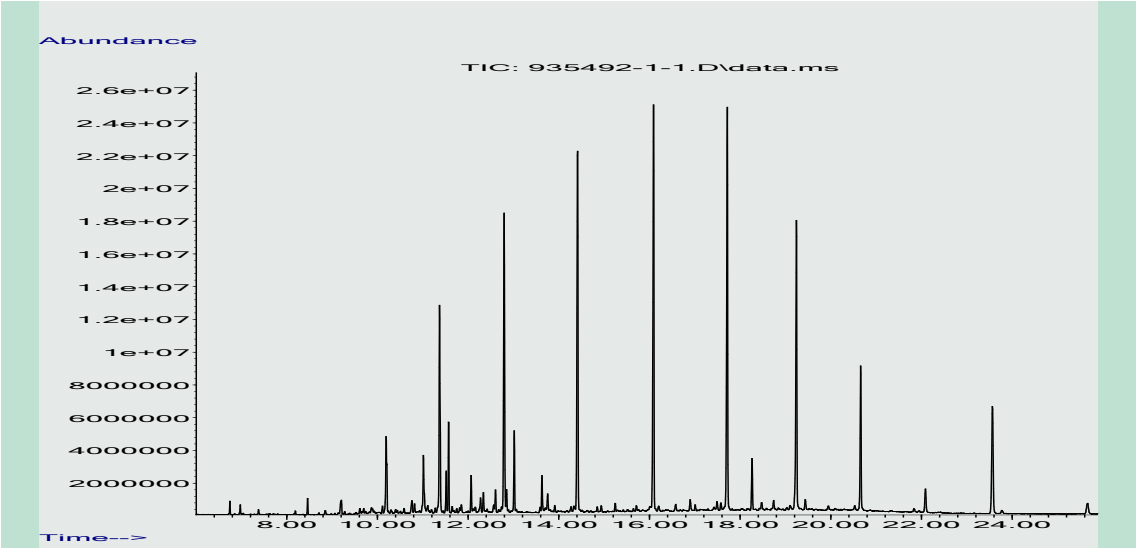

FIGURE 25 GC/MS chromatography for screening of sample 1.1. Note that unit scale is normalized for comparison with other GC/MS chromatography analyses.

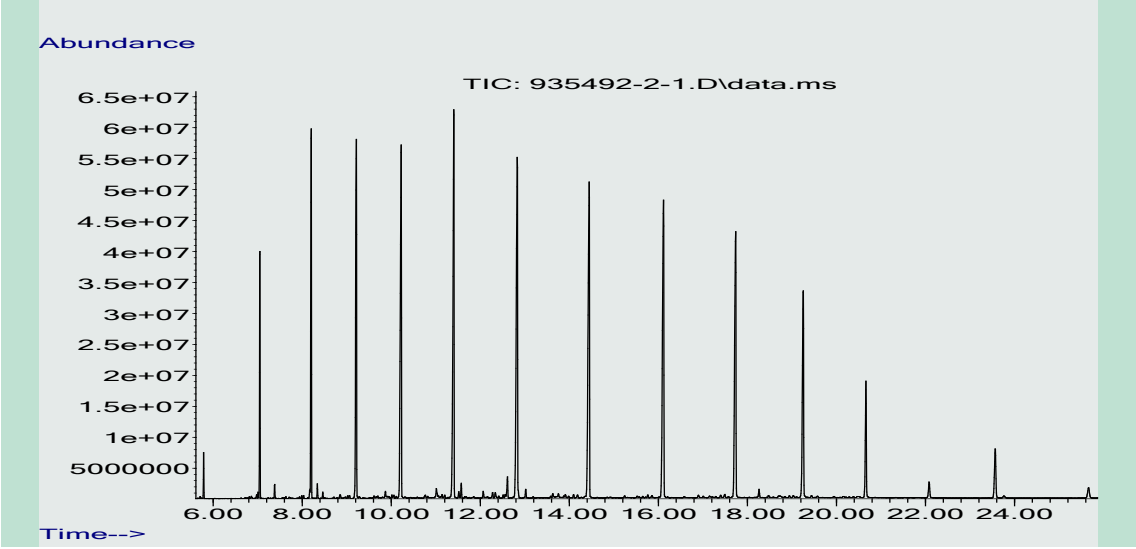

FIGURE 26 GC/MS chromatography for screening of sample 2.1. Note that unit-scale is normalized for comparison with other GC/MS chromatography analyses.

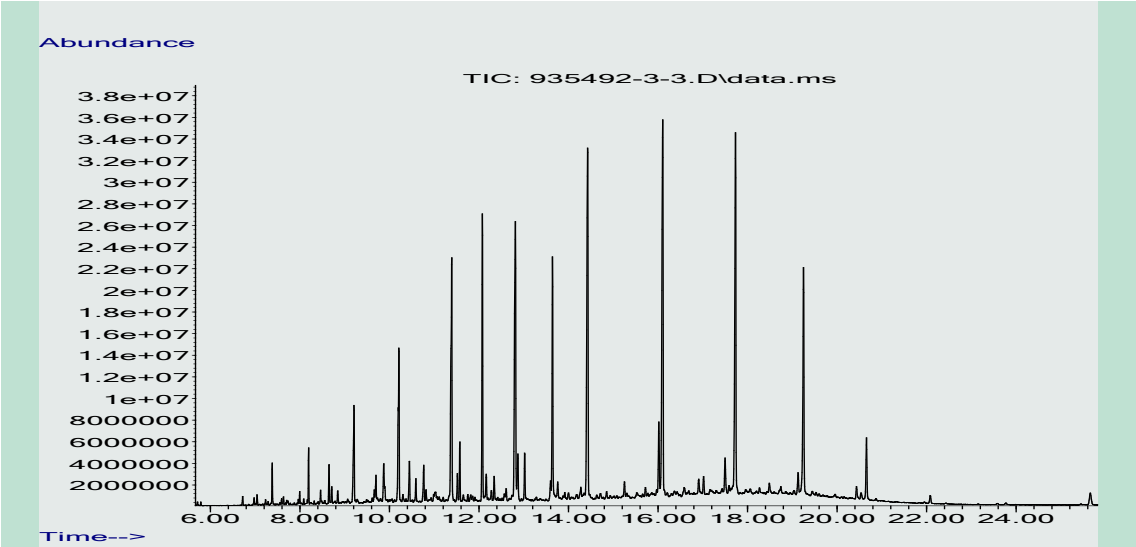

FIGURE 27 GC/MS chromatography for screening of sample 3.3. Note that unit-scale is normalized for comparison with other GC/MS chromatography analyses.

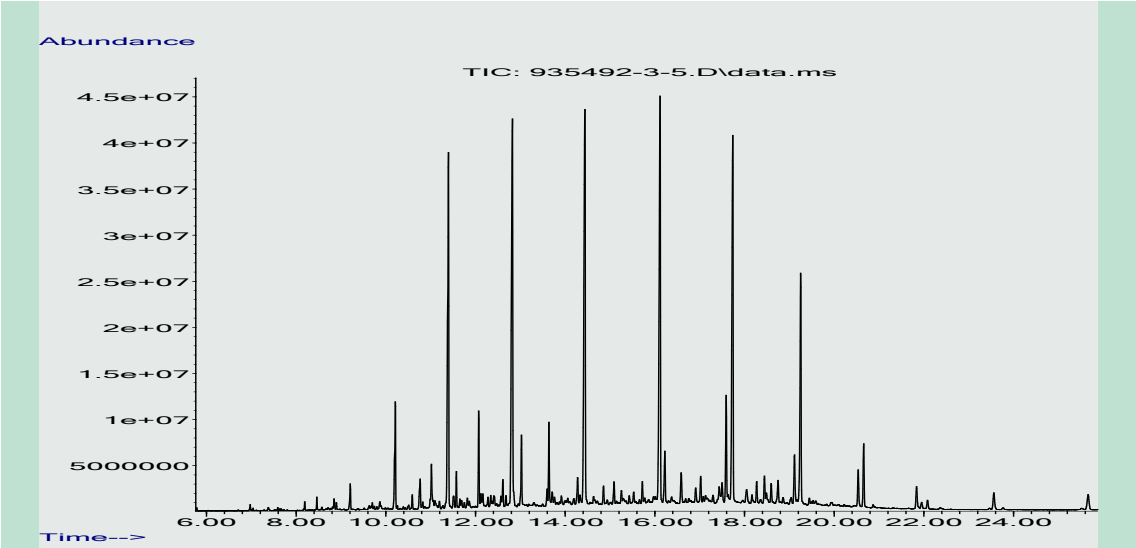

FIGURE 28 GC/MS chromatography for screening of sample 3.5. Note that unit-scale is normalized for comparison with other GC/MS chromatography analyses.

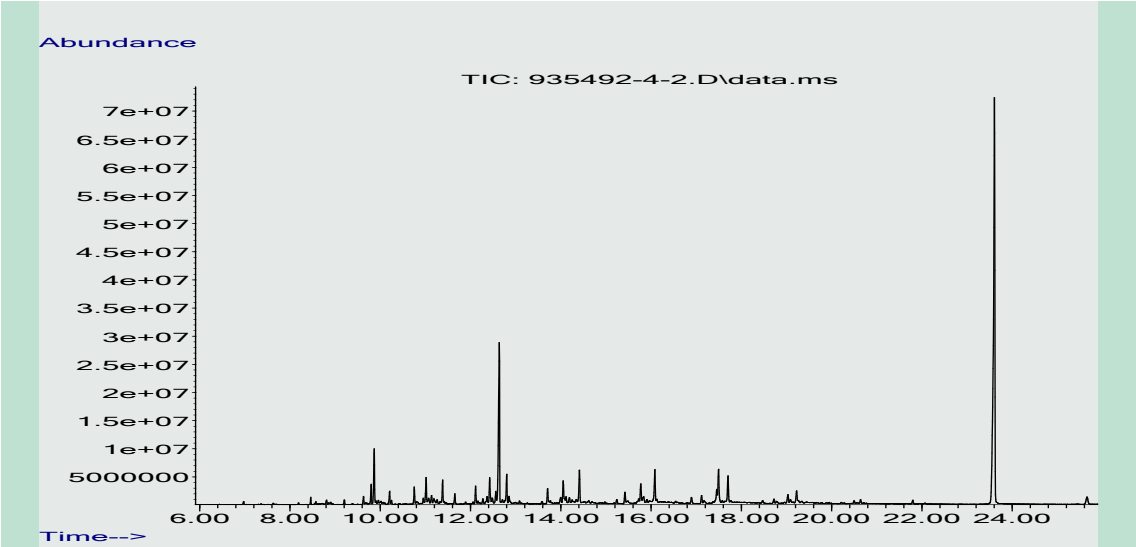

FIGURE 29 GC/MS chromatography for screening of sample 4.2. Note that unit-scale is normalized for comparison with other GC/MS chromatography analyses.

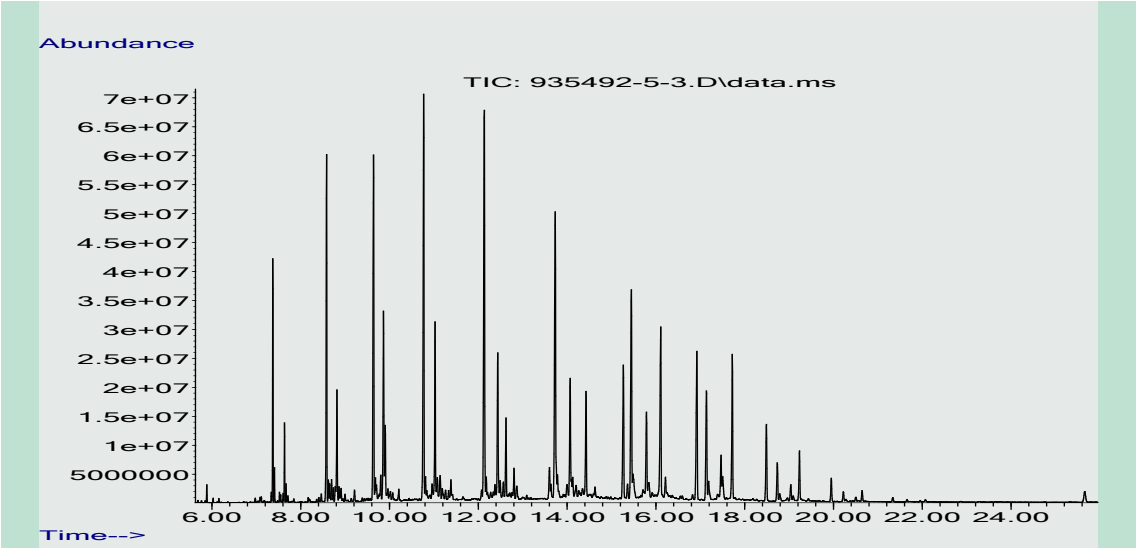

FIGURE 30 GC/MS chromatography for screening of sample 5.3. Note that, unit-scale is normalized for comparison with other GC/MS chromatography analyses.

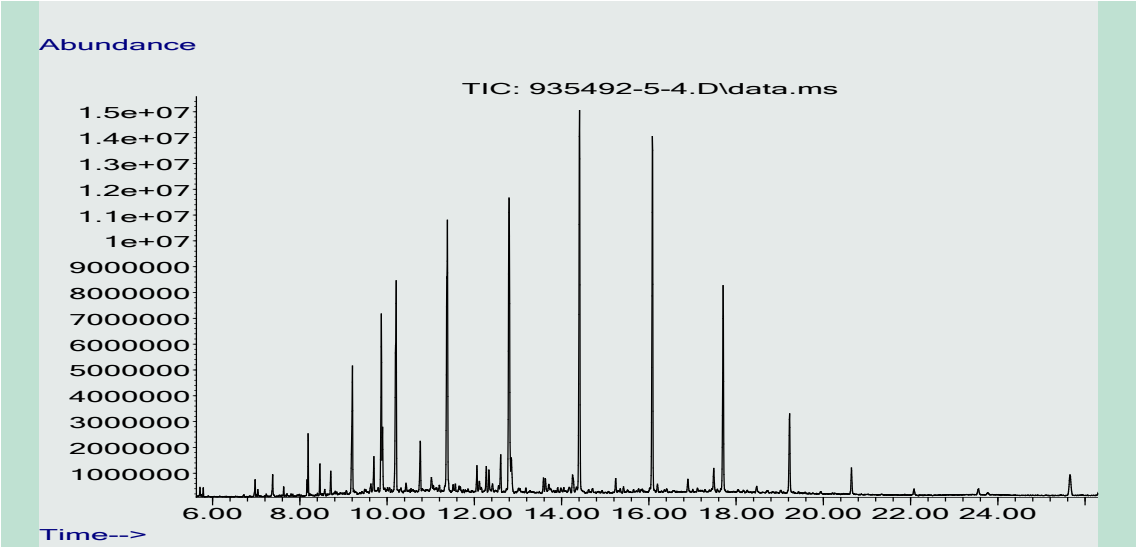

FIGURE 31 GC/MS chromatography for screening of sample 5.4. Note that unit-scale is normalized for comparison with other GC/MS chromatography analyses.

TABLE 34 GC/MS screening of sample 1.1. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 1.1)	RT [min]	CAS No.	Concentration* [mg/kg]
1-Butoxy-2-propanol	6.748	5131-66-8	5.8
Not identified, co-elution, may be saturated and unsaturated alkane	9.206	-	13
Not identified, could be Indan-1,3-diol monopropionate	10.112	(none available)	4.3
Not identified, co-elution, may be saturated and unsaturated alkane	10.195	-	62
Not identified, could be saturated alkane	10.764	-	10
Methyl dihydrojasmonate	10.818	24851-98-7	5.0
n-Hexyl salicylate	11.017	6259-76-3	42
Not identified	11.110	-	3.8
Not identified, could be 1-nonadecene and octadecane	11.373	(18435-45-5 and 593-45-3)	150
alpha-Hexylcinnamaldehyde	11.519	101-86-0	21
Isopropyl myristate	11.572	110-27-0	43
Not identified	11.855	-	3.8
Not identified, could be Hexadecanol	12.069	36653-82-4	19
Hexadecenoic acid, methyl ester	12.337	112-39-0	11
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.605	82304-66-3	11
Not identified, co-elution, Eicosene (C22:1) and saturated alkane, could be eicosane (C20)	12.794	(1599-67-3 and 112-95-8)	200
Isopropyl palmitate	13.018	142-91-6	44
Not identified, could be Eicosanol	13.632	(629-96-9)	20
Not identified, could be Methyl octadecenoate	13.758	(13481-95-3)	10
Methyl stearate	13.914	112-61-8	4.3
Octadecenoic acid ethyl ester	14.274	6114-18-7	4.2

Component (Sample no. 1.1)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, could be docosene; co-elution may be present	14.416	1599-67-3	260
Tributyl acetyl citrate	14.937	77-90-7	4.5
Not identified, saturated alkane	15.248	-	5.2
1-Tetracosene (C24:1)	16.090	10192-32-2	280
Not identified, ester of benzoic acid and saturated alcohol, could be benzoic acid, tetradecyl ester	16.577	70682-72-3	5.7
Not identified, saturated alkane	16.899	-	9.0
Octan-2-yl palmitate	17.011	55194-81-5	4.2
Not identified, could be diethylhexyl phthalate	17.493	117-81-7	5.6
Not identified, could be Dodecanoic acid, dodecyl ester	17.580	(13945-76-1)	5.4
Not identified, could be hexacosene (C26:1)	17.717	(18835-33-1)	280
Bumetrizole	18.267	3896-11-5	34
Not identified, linear alkane, possible heptacosane	18.476	(593-49-7)	4.4
Octocrylene	18.739	6197-30-4	7.0
Not identified, ester, could be dodecanoic acid, tetradecyl ester	19.104	(22412-97-1)	4.3
Not identified, linear alcohol, could be octacosanol	19.245	(557-61-9)	210
Squalene	19.440	111-02-4	7.8
Not identified, could be triacontene (C30:1)	20.662	-	96
Not identified, could be dotriaconene (C32:1)	22.089		20
Tris-(2,4-di-t-butylphenyl) phosphite	23.569	31570-04-4	110
Not identified, likely phenol compound	25.667	-	14

TABLE 35 GC/MS screening of sample 2.1. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 2.1)	RT [min]	CAS No.	Concentration* [mg/kg]
Octane	5.788	111-65-9	39
Decene	7.010	872-05-9	5.8
Decane	7.049	124-18-5	269.0
Limonene	7.380	138-86-3	15
Dodecane	8.203	112-40-3	520
2-Propylheptanol	8.340	10042-59-8	16
Not identified, co-elution, could be Isobornyl acetate and tert-Butylcyclohexyl acetate	8.851	(125-12-2 and 88-41-5)	7.0
3-Methyltridecane	9.065	6418-41-3	4.3
Tetradecane (C14)	9.216	629-59-4	700
2,4-Di-tert-butylphenol	9.868	96-76-4	6.9
Not identified, saturated alkane	10.058	-	4.0
Hexadecane (C16)	10.224	544-76-3	790
Not identified, saturated alkane	10.764	-	6.8
n-Hexyl salicylate	11.017	6259-76-3	16
Not identified, saturated alkane	11.202	-	5.5
Octadecane (C18)	11.407	593-45-3	850
alpha-Hexylcinnamaldehyde	11.519	101-86-0	8.8
Isopropyl myristate	11.572	110-27-0	20
Not identified, likely branched alcohol, could be 2-Hexyl-1-decanol	12.069	(2425-77-6)	11
Hexadecanoic acid, methyl ester	12.337	112-39-0	9.3
Not identified, saturated branched alkane, could be 2-Methylnonadecane	12.517	(1560-86-7)	4.6
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.609	82304-66-3	32
Eicosane (C20)	12.833	112-95-8	890
Isopropyl palmitate	13.023	142-91-6	13
Not identified, alcohol, could be octadecanol	13.627	(112-92-5)	6.6
Not identified, likely Methyl 10-octadecenoate	13.753	(13481-95-3)	5.2
Methyl stearate	13.914	112-61-8	3.9
Not identified, saturated alkane (branched)	14.094	-	5.9
Not identified, saturated alkane	14.187	-	7.4
Docosane (C22)	14.445	629-97-0	860
Not identified, saturated alkane	15.764	-	5.6
Not identified, saturated alkane (branched)	15.857	-	6.1
Tetracosane (C24)	16.115	646-31-1	800
Not identified, saturated alkane	16.899	-	6.3

Component (Sample no. 2.1)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, saturated alkane	17.152	-	4.2
Not identified, saturated alkane	17.400	-	5.3
Not identified, possibly ortho or terephthalate	17.493	-	7.8
Hexacosane (C26)	17.736	630-01-3	710
Bumetrizole	18.262	3896-11-5	15
Not identified, saturated alkane	18.943	-	4.3
Not identified, saturated alkane	19.031	-	5.2
Octacosane (C28)	19.255	630-02-4	510
Squalene	19.440	111-02-4	4.6
Triacontane (C30)	20.662	638-68-6	230
Dotriacontane (C32)	22.084	544-85-4	41
Tris-(2,4-di-t-butylphenyl) phosphite	23.569	31570-04-4	140
Tetratriacontane (C34)	23.759	14167-59-0	7.2
Not identified	25.667	-	38

*: Calculated as naphthalene equivalents

(): CAS numbers in parenthesis are related to suggested compound(s)

N/A: No CAS number is available for the component

TABLE 36 GC/MS screening of sample 3.3. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 3.3)	RT [min]	CAS No.	Concentration* [mg/kg]
α-Pinene	6.723	80-56-8	6.4
Co-elution, decane (C10) and β-pinene	7.045	124-18-5 and 127-91-3	7.3
Limonene	7.380	138-86-3	24
Undecane (C11)	7.634	1120-21-4	4.5
o-Cymene (or isomer)	7.994	527-84-4	6.9
Isophorone	8.086	78-59-1	3.8
Dodecane (C12)	8.193	112-40-3	30
1-Decanol	8.651	112-30-1	30
Tridecane (C13)	8.710	629-50-5	12
tert-Butyl cyclohexyl acetate	8.846	88-41-5	11
Tetradecane (C14)	9.211	629-59-4	100
Not identified, could be undecanol	9.664	(112-42-5)	5.0
Pentadecane (C15)	9.698	629-62-9	16.5
2,4-Di-tert-butylphenol	9.873	96-76-4	24
Butylated Hydroxytoluene	9.885	128-37-0	10
Hexadecane (C16)	10.214	544-76-3	170
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB)	10.302	6846-50-0	7.0
Diethyl Phthalate	10.448	84-66-2	35
Octyl ether	10.589	629-82-3	17
Heptadecane (C17)	10.769	629-78-7	33
Methyl (3-oxo-2-pentylcyclopentyl)acetate (hedione)	10.818	24851-98-7	9.4
Co-elution, octadecene and octadecane	11.392	7206-25-9, 593-45-3	300
alpha-Hexylcinnamaldehyde	11.519	101-86-0	23
Isopropyl myristate	11.572	110-27-0	43
Not identified, could be 3,5-di-tert-Butyl-4-hydroxybenzaldehyde	11.650	(1620-98-0)	4.9
Benzyl Benzoate	11.752	120-51-4	5.9
2-Ethylhexyl salicylate	11.816	118-60-5	5.6
Not identified, could be hexadecanol	12.079	(36653-82-4)	230
Versalide	12.161	88-29-9	21
Hexadecanoic acid, methyl ester	12.342	112-39-0	21
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.609	82304-66-3	9.1
Co-elution, aliphatic alcohol and eicosane (C20)	12.814	(112-95-8)	370
Isopropyl palmitate	13.023	142-91-6	38.5
Aliphatic alcohol or unsaturated alkane	13.646	-	200
Methyl elaidate (double bond may be different position)	13.758	112-62-9	14
Methyl stearate	13.919	11261-8	4.0
Oxybenzone	14.002	131-57-7	7.4
Not identified, saturated aliphatic	14.182	-	6.4

Component (Sample no. 3.3)	RT [min]	CAS No.	Concentration* [mg/kg]
Ethyl Oleate	14.279	111-62-6	13
Docosene (C22:1)	14.430	1599-67-3	470
Not identified, could be Behenic alcohol	14.717	(661-19-8)	7.4
Ester of benzoic acid, may be benzoic acid, undecyl ester	14.854	(6316-30-9)	7.9
Not identified, saturated aliphatic	15.253	-	15
Not identified, saturated aliphatic	15.526	-	6.3
Ester of benzoic acid, may be benzoic acid, undecyl ester	15.720	(6316-30-9)	8.9
Not identified	15.862	-	4.4
Octinoxate	16.017	5466-77-3	64.2
Tetracosene (C24:1)	16.105	10192-32-2	490
Not identified, unsaturated aliphatic compound	16.368	-	5.6
Not identified, saturated aliphatic	16.426	-	4.4
Ester of benzoic acid, may be benzoic acid, hexadecyl ester	16.587		14
Not identified, saturated aliphatic	16.908	-	15
Octan-2-yl palmitate	17.020	55194-81-5	19
Bis(2-ethylhexyl) phthalate (DEHP)	17.497	117-81-7	42
Dodecanoic acid, dodecyl ester	17.590	13945-76-1	6.5
Hexacosene (C26:1)	17.731	18835-33-1	450
Not identified, unsaturated aliphatic compound	18.062	-	5.1
Bumetrizole	18.267	3896-11-5	5.8
Not identified, saturated aliphatic	18.491	-	11
Octocrylene	18.744	6197-30-4	11
Not identified	19.036	-	4.8
Hexadecanoic acid, decyl ester	19.133	42232-27-9	22
Not identified, could be octacosene (C28:1) or octadecanol	19.250	(557-61-9)	270
Not identified	19.956	-	4.3
Not identified	20.433	-	16
Not identified, ester-compound	20.535	-	8.8
Not identified, unsaturated aliphatic compound or alcohol	20.657	-	69
Not identified, unsaturated aliphatic or alcohol	22.084	-	11
Not identified, phenol compound	25.657	-	24

*: Calculated as naphthalene equivalents

(): CAS numbers in parenthesis are related to suggested compound(s)

N/A: No CAS number is available for the component

TABLE 37 GC/MS screening of sample 3.5. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 3.5)	RT [min]	CAS No.	Concentration* [mg/kg]
Dodecane (C12)	8.193	112-40-3	4.1
tert-Butyl cyclohexyl acetate	8.846	88-41-5	6.5
2,2,4,4,6,8,8-Heptamethylnonane	8.899	4390-04-9	4.3
Tetradecane (C14)	9.206	629-59-4	19
Not identified, saturated alkane	9.698	-	3.4
2,4-Di-tert-butylphenol	9.868	96-76-4	4.0
Hexadecane (C16)	10.214	544-76-3	94
Octyl ether	10.589	629-82-3	10
Co-elution, Heptadecane (C17) and aromatic compounds, could be 3-Phenylundecane	10.764	629-78-7 and (4536-87-2)	29
Not identified, aldehyde, could be 2-Formylhexadecane	10.823	(55019-46-0)	4.3
n-Hexyl salicylate	11.017	6259-76-3	25
5-Phenyldodecane	11.095	2719-63-3	2.7
4-Phenyldodecane	11.197	2719-64-4	4.8
Not identified	11.275	-	3.0
Octadecane (C18)	11.397	593-45-3	360
Co-elution, Carbonic acid, bis(2-ethylhexyl) ester and alpha-Hexylcinnamaldehyde	11.514	14858-73-2 and 101-86-0	12
Isopropyl myristate	11.572	110-27-0	20
2-Phenyldodecane	11.655	2719-61-1	4.5
6-Phenyltridecane	11.689	4534-49-0	4.3
5-Phenyltridecane	11.752	4534-50-3	3.8
2-Ethylhexyl salicylate	11.821	118-60-5	6.5
4-Phenyltridecane	11.864	4534-51-4	3.8
1-Hexadecanol	12.074	36653-82-4	60
Not identified	12.118	-	5.8
Versalide	12.166	88-29-9	7.5
Hexadecanoic acid, methyl ester	12.342	112-39-0	6.7
Not identified	12.410	-	9.2
Not identified, likely Methyl 3-(3,5-di-tert-butyl-4-hydroxy-phenyl)propionate	12.570	6386-38-5	4.4
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.609	82304-66-3	17
Not identified	12.682	-	7.7
Eicosane (C20)	12.824	112-95-8	460
Isopropyl palmitate	13.028	142-91-6	53
Not identified, saturated alkane	13.598	-	6.9
Not identified, aliphatic alcohol or alkene	13.637	-	51
Not identified, saturated alkane	13.710	-	8.5
Not identified, could be 10-Octadecenoic acid, methyl ester	13.763	13481-95-3	5.0
Methyl stearate	13.914	112-61-8	6.8
Not identified	14.060	-	3.0

Component (Sample no. 3.5)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, saturated alkane	14.192	-	6.6
Ethyl Oleate	14.279	111-62-6	24
Octanoic acid, dodecyl ester	14.328	20292-09-5	7.6
Docosane (C22)	14.440	629-97-0	490
Oleamide (may be different chain length)	14.635	301-02-0	3.5
Not identified, could be Benzoic acid, pentadecyl ester	14.854	(1000340-22-8)	15
Co-elution, Tributyl acetylcitrate and saturated alkane	14.941	77-90-7	3.9
Not identified	15.019	-	3.1
n-Propyl 11-octadecenoate	15.092	1000336-71-7	20
Not identified, saturated alkane	15.253	-	9.2
Not identified, saturated alkane	15.297	-	3.2
Not identified, saturated alkane	15.428	-	5.9
Not identified, saturated alkane	15.531	-	9.6
Not identified, saturated alkane	15.657	-	3.4
Not identified, could be Benzoic acid, hexadecyl ester	15.720	N/A	16
Not identified, saturated alkane	15.774	-	3.6
Not identified, saturated alkane	15.862	-	4.0
Not identified	15.974	-	3.2
Tetracosane (C24)	16.115	646-31-1	470
Oleamide (may be different chain length)	16.222	301-02-0	50
Not identified, could be 3-Octadecanone	16.373	-	3.9
Not identified, aromatic alkane, could be Benzoic acid, octadecyl ester	16.587	10578-34-4	31
Piperonyl butoxide	16.689	51-03-6	2.8
Not identified	16.757	-	2.7
Not identified, saturated alkane	16.913	-	14.1
Octan-2-yl palmitate	17.020	55194-81-5	22
Not identified, could be Didodecyldimethylammonium (unknown anion)	17.079	3282-73-3	4.2
Not identified, saturated alkane	17.132	-	3.5
Not identified, could be Hexanoic acid, 3,5,5-trimethyl-, hexadecyl ester	17.298	N/A	7.3
Aromatic alkane, could be benzoic acid, pentadecyl ester	17.434	N/A	7.2
Diethylhexyl phthalate (DEHP)	17.497	74746-55-7	14
Dodecanoic acid, dodecyl ester	17.590	13945-76-1	84
Hexacosane (C26)	17.736	630-01-3	390
Not identified, likely co-elution and saturated alkane	17.960	-	2.9
Not identified, saturated alkane	18.048	-	17
Not identified	18.169	-	7.3
Bumetrizole	18.272	3896-11-5	18
Not identified, could be aliphatic ester	18.359	-	4.6
Not identified, could be aliphatic ester	18.442	-	20
Not identified, saturated alkane	18.491	-	6.0
Not identified, could be aliphatic ester	18.593	-	16

Component (Sample no. 3.5)	RT [min]	CAS No.	Concentration* [mg/kg]
Octocrylene	18.749	6197-30-4	23
Not identified, saturated alkane	18.861	-	6.1
Not identified, saturated alkane	19.041	-	8.6
Tetradecanoic acid, dodecyl ester	19.114	2040-64-4	45
Not identified, could be ether compound and trace of DEHP	19.255	-	220
Squalene	19.445	111-02-4	4.8
Not identified, could be ortho-phthalate	19.591	-	3.0
Hexadecanoic acid, dodecyl ester	20.535	42232-29-1	35
Not identified, likely saturated alkane	20.657	-	56
Not identified, could be Oleic acid, 2-(1-octade-cenyloxy)ethyl ester but likely smaller molecule	20.867	30760-07-7	2.7
Not identified, could be Decyl oleate	21.835	3687-46-5	26
Not identified, could be Octadecanoic acid, octadecyl ester	21.952	2778-96-3	7.3
Not identified	22.079	-	9.4
Tris-(2,4-di-t-butylphenyl) phosphite	23.559	31570-04-4	22
Not identified, likely saturated alkane	23.768	-	2.7
Not identified	25.662	-	25

*: Calculated as naphthalene equivalents

(): CAS numbers in parenthesis are related to suggested compound(s)

N/A: No CAS number is available for the component

TABLE 38 GC/MS screening of sample 4.2. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 4.2)	RT [min]	CAS No.	Concentration* [mg/kg]
Decane, 2,3,5,8-tetramethyl-	8.812	192823-15-7	5.8
Tetradecane (C14)	9.206	629-59-4	6.7
Not identified, saturated alkane	9.634	-	10
2,6-Di-tert-butylbenzoquinone	9.800	719-22-2	27
2,4-Di-tert-butylphenol	9.868	96-76-4	84
Not identified, saturated alkane	9.961	-	4.1
Hexadecane (C16)	10.209	-	16
Not identified, aromatic compound	10.253	-	4.7
Heptadecane (C17)	10.754	629-78-7	22
Not identified, possibly aliphatic alcohol	10.959	-	6.5
Not identified, saturated alkane	11.017	-	37
Not identified, aliphatic compound	11.076	-	8.1
Not identified, aliphatic compound	11.139	-	12
Not identified, aliphatic compound	11.192	-	9.9
Not identified, aliphatic compound	11.265	-	5.0
Not identified, aliphatic compound	11.382	-	29
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	11.655	1620-98-0	15.6
Not identified, aliphatic compound	12.113	-	25
Not identified, aliphatic alcohol or ether compound	12.366	-	12
Not identified	12.429	-	38
Not identified, saturated alkane	12.483	-	6.8
Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	12.565	6386-38-5	14
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.638	82304-66-3	310
Not identified	12.711	-	3.7
Eicosane (C20)	12.804	112-95-8	40
Not identified, saturated alkane	13.086	-	3.5
Not identified, saturated alkane	13.588	-	4.3
Not identified, saturated alkane	13.710	-	24
Not identified, may be aliphatic alcohol	14.002	-	11
Not identified, saturated alkane	14.055	-	29
Not identified, saturated alkane	14.118	-	4.5
Not identified, saturated alkane	14.192	-	9.4
Not identified, saturated alkane	14.347	-	3.6
Not identified, saturated alkane	14.415	-	55
Not identified, saturated alkane	15.243	-	7.3
Not identified, saturated alkane	15.423	-	18
Not identified, saturated alkane	15.774	-	27
Not identified, saturated alkane	15.837	-	11
Not identified, saturated alkane	15.910	-	5.5
Tetracosane (C24)	16.085	646-31-1	55
Pentacosane (C25)	16.898	629-99-2	12
Not identified, saturated alkane	17.122	-	13

Component (Sample no. 4.2)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, saturated alkane	17.176	-	6.3
Not identified, saturated alkane	17.458	-	7.3
Bis(2-ethylhexyl) phthalate	17.497	117-81-7	44
Not identified, saturated alkane	17.707	-	47
Not identified, saturated alkane	18.476	-	4.9
Not identified, saturated alkane	18.724	-	8.4
Not identified	18.783	-	4.6
Not identified	19.036	-	17
Not identified	19.089	-	5.9
Not identified, saturated alkane	19.226	-	20
Not identified, saturated alkane	20.501	-	5.4
Not identified, saturated alkane	20.642	-	6.1
Not identified, may be related to Bis(2,2,6,6-tetramethyl-4-piperidinyl) sebacate	21.801	(52829-07-9)	7.3
Tris-(2,4-di-t-butylphenyl) phosphite	23.612	31570-04-4	1000
Not identified	25.662	-	25

TABLE 39 GC/MS screening of sample 5.3. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 5.3)	RT [min]	CAS No.	Concentration* [mg/kg]
2,4-Dimethylheptane or isomer	5.886	2213-23-2	12
2,4-Dimethyl-1-heptene or isomer	6.027	19549-87-2	3.0
4-Methyloctane or isomer	6.158	2216-34-4	3.0
Not identified, aliphatic compound	7.113	-	3.2
Not identified, aliphatic compound	7.337	-	5.4
Not identified, aliphatic compound	7.375	-	170
Not identified, aliphatic compound	7.410	-	22
Not identified, aliphatic compound, may be unsaturated	7.522	-	5.1
Not identified, aliphatic compound, may be unsaturated	7.551	-	4.8
Not identified, aliphatic compound	7.609	-	5.6
Not identified, aliphatic compound	7.638	-	48
Not identified, aliphatic compound	7.672	-	11
Not identified, aliphatic compound	7.711	-	5.2
Aliphatic compound, may be unsaturated	8.169	-	2.6
Not identified, aliphatic compound	8.198	-	2.9
Not identified, aliphatic compound	8.408	-	3.8
Not identified, aliphatic compound, could be 2,6,11-Trimethyl-dodecane or similar	8.583	(31295-56-4)	320
Not identified, aliphatic compound	8.627	-	14
Not identified, aliphatic compound	8.656	-	12
Not identified, aliphatic compound	8.695	-	15
Not identified, aliphatic compound, may be unsaturated	8.734	-	10
Not identified, aliphatic compound	8.783	-	5.0
Not identified, aliphatic compound, could be 2,6,11-Trimethyl-dodecane or similar	8.817	(31295-56-4)	92
Not identified, aliphatic compound	8.865	-	10
Not identified, aliphatic compound	8.909	-	10
3,5,5-Trimethyl-2(5H)-furanone	9.002	50598-50-0	6.8
Not identified	9.138	-	3.6
Not identified, could be aliphatic alcohol	9.216	-	12
Aliphatic aldehyde, could be undecanal	9.391	(112-44-7)	3.1
Not identified, aliphatic compound	9.571	-	2.6
Aliphatic compound, could be pentadecane (C15)	9.644	(629-62-9)	390
Not identified, aliphatic compound	9.683	-	9.4
Not identified, aliphatic compound	9.805	-	20
Co-elution, aliphatic compound and 2,4-Di-tert-butylphenol	9.868	(96-76-4)	160
Butylated Hydroxytoluene	9.907	128-37-0	51
Not identified, aliphatic compound	9.966	-	5.5
Not identified, aliphatic compound	10.024	-	6.2
Not identified, aliphatic compound	10.073	-	7.4
Not identified, aliphatic compound	10.214	-	11

Component (Sample no. 5.3)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, aliphatic compound	10.774	-	450
Not identified, aliphatic compound	10.813	-	14
Not identified, aliphatic compound	10.842	-	4.2
Not identified, aliphatic compound	10.915	-	5.4
Not identified	10.964	-	13
Not identified, aliphatic compound	11.027	-	160
Not identified, aliphatic compound	11.076	-	17
Not identified, aliphatic compound	11.139	-	31
Not identified	11.188	-	8.7
Not identified, could be ether compound	11.265	-	8.1
Not identified, aliphatic compound	11.334	-	6.7
Not identified	11.387	-	15
Not identified, aliphatic compound	12.079	-	7.6
Not identified, aliphatic compound	12.137	-	510
Not identified, aliphatic compound	12.181	-	13
Not identified	12.341	-	4.0
Not identified, aliphatic compound	12.376	-	9.8
Not identified, aliphatic compound	12.439	-	160
Not identified	12.565	-	17
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.624	82304-66-3	81
Not identified, aliphatic compound	12.711	-	3.8
Not identified, aliphatic compound	12.765	-	3.5
Not identified, aliphatic compound	12.809	-	29.6
Not identified, aliphatic compound	13.091	-	4.1
Not identified, aliphatic compound	13.602	-	21
Not identified, aliphatic compound	13.637	-	5.7
Not identified, aliphatic compound	13.734	-	400
Not identified, aliphatic compound	13.787	-	8.8
Not identified, aliphatic compound	14.002	-	19
Not identified, aliphatic compound	14.070	-	120
Not identified, aliphatic compound	14.128	-	9.6
Not identified, aliphatic compound	14.206	-	19
Not identified, aliphatic compound	14.265	-	5.0
Not identified, aliphatic compound	14.347	-	9.6
Not identified, aliphatic compound	14.430	-	130
Not identified, aliphatic compound	14.630	-	9.7
Not identified, aliphatic compound	14.771	-	3.1
Not identified, aliphatic compound	15.268	-	180
Not identified	15.365	-	19
Not identified, aliphatic compound	15.448	-	270
Not identified, aliphatic compound	15.487	-	12
Not identified, aliphatic compound	15.711	-	4.9
Not identified, aliphatic compound	15.788	-	100

Component (Sample no. 5.3)	RT [min]	CAS No.	Concentration* [mg/kg]
Not identified, aliphatic compound	15.842	-	17
Not identified, aliphatic compound	15.920	-	6.2
Tetracosane (C24)	16.110	646-31-1	240
Octadecenamide or isomer	16.217	(301-02-0)	18
Octadecenamide or isomer	16.373	(301-02-0)	2.7
Not identified, aliphatic compound	16.553	-	3.4
Not identified, aliphatic compound	16.597	-	3.4
Tetraethylene glycol di-2-ethylhexoate	16.830	18268-70-7	7.3
Not identified, aliphatic compound	16.923	-	220
Not identified, aliphatic compound	17.142	-	150
Not identified, aliphatic compound	17.191	-	22
Not identified, aliphatic compound	17.390	-	6.5
Not identified, aliphatic compound	17.468	-	37
Bis(2-ethylhexyl) phthalate	17.507	117-81-7	10
Not identified, aliphatic compound	17.726	-	180
Not identified, aliphatic compound	18.271	-	2.9
Not identified, aliphatic compound	18.491	-	100
Not identified, aliphatic compound	18.739	-	49
Not identified, aliphatic compound	18.792	-	10
Not identified, aliphatic compound	18.968	-	6.6
Not identified, aliphatic compound	19.041	-	22
Not identified	19.094	-	5.9
Not identified, aliphatic compound	19.235	-	60
Not identified	19.440	-	3.4
Not identified, aliphatic compound	19.951	-	30
Not identified, aliphatic compound	20.224	-	13
Not identified, aliphatic compound	20.287	-	3.1
Not identified, aliphatic compound	20.506	-	6.1
Not identified, aliphatic compound	20.647	-	14
Not identified, aliphatic compound	21.339	-	6.8
Not identified, aliphatic compound	21.660	-	3.4
Not identified, aliphatic compound	22.074	-	3.6
Not identified	25.662	-	26

*: Calculated as naphthalene equivalents

(): CAS numbers in parenthesis are related to suggested compound(s)

N/A: No CAS number is available for the component

TABLE 40 GC/MS screening of sample 5.4. Results are expressed as [mg] analyte per [kg] product simulant.

Component (Sample no. 5.4)	RT [min]	CAS No.	Concentration* [mg/kg]
Limonene	7.380	138-86-3	6.8
Dodecane (C12)	8.193	112-40-3	12
Tridecane (C13)	8.709	629-50-5	6.5
Tetradecane (C14)	9.206	629-59-4	46
Pentadecane (C15)	9.698	629-62-9	10
2,4-Di-tert-butylphenol	9.868	96-76-4	37
Butylated Hydroxytoluene	9.897	128-37-0	5.8
Hexadecane (C16)	10.209	544-76-3	87
Heptadecane (C17)	10.764	629-78-7	18
Not identified	11.017	-	5.3
Co-elution, Octadecane (C18) and unsaturated alkane	11.382	593-45-3	130
Nonedecane (C19)	12.059	-	8.0
Hexadecanoic acid, methyl ester	12.336	112-39-0	6.9
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	12.604	82304-66-3	11
Not identified	12.799	-	130
Alkane	13.588	-	4.6
Not identified	13.627	-	4.7
Not identified, could be aliphatic alcohol	14.177	-	3.4
Ethyl Oleate	14.255	111-62-6	9.7
Not identified, co-elution, could be alkane and alkene	14.411	-	150
Saturated aliphatic	15.243	-	5.1
Not identified	16.085	-	130
Not identified, aliphatic compound	16.898	-	5.1
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (DEHP)	17.488	74746-55-7	8.4
Not identified	17.702	-	74
Unsaturated aliphatic compound	19.226	-	31
Unsaturated aliphatic compound	20.647	-	9.7
Tris-(2,4-di-t-butylphenyl) phosphite	23.559	31570-04-4	3.8
Not identified	25.657	-	16
Not identified	26.329	-	3.6

Appendix 5: LC/MS multitarget components

TABLE 41 Overview of compounds examined by LC/MS multitarget analysis and their associated detection limits. Results are expressed as [mg] analyte per [kg] product simulant.

Component	CAS No.	Detection limit [mg/kg]
Primary aromatic amines		
4-Aminoazobenzene	60-09-3	0.002 mg/kg
2-Aminonaphthalene	91-59-8	0.01 mg/kg
3,3'-Dichlorobenzidine	91-94-1	0.1 mg/kg
4-Aminobiphenyl	92-67-1	0.05 mg/kg
Benzidine	92-87-5	0.01 mg/kg
4-Chloro-o-toluidine	95-69-2	0.1 mg/kg
2,4-Diaminotoluene	95-80-7	0.01 mg/kg
4-Amino-2'-3-dimethylazobenzene	97-56-3	0.002 mg/kg
4,4'-Methylene-bis-(2-chloraniline)	101-14-4	0.1 mg/kg
4,4'-Diaminodiphenylmethane	101-77-9	0.01 mg/kg
4,4'-Oxydianiline	101-80-4	0.01 mg/kg
p-Chloroaniline	106-47-8	0.1 mg/kg
3,3'-Dimethoxybenzidine	119-90-4	0.002 mg/kg
3,3'-Dimethylbenzidine	119-93-7	0.002 mg/kg
p-Cresidine	120-71-8	0.01 mg/kg
2,4,5-Trimethylaniline	137-17-7	0.002 mg/kg
4,4'-Thioaniline	139-65-1	0.01 mg/kg
2,4-Diaminoanisole	615-05-4	0.002 mg/kg
3,3'-Dimethyl-4,4'-diaminodiphenylmethane	838-88-0	0.002 mg/kg
Monomers		
Benzoguanamine	91-76-9	0.01 mg/kg
Hexamethylenetetramine	100-97-0	0.01 mg/kg
Isophoronediamine	2855-13-2	0.01 mg/kg
Melamine	108-78-1	0.01 mg/kg
1,6-Hexanediol diacrylate	13048-33-4	0.01 mg/kg
1,6-Diaminohexane	124-09-4	0.01 mg/kg
Sebacic acid	111-20-6	0.01 mg/kg
ε-Caprolactam	105-60-2	0.01 mg/kg
Perfluortensides		
Pentadecafluorooctanoic acid	335-67-1	0.01 mg/kg
Perfluorooctanesulfonic acid, PFOA	1763-23-1	0.01 mg/kg

Component	CAS No.	Detection limit [mg/kg]
UV- Photoinitiators		
4,4'-Bis(diethylamino)benzophenone (Dublecure EMK)	90-93-7	0.01 mg/kg
4,4'-Bis(dimethylamino)benzophenone (Michler's Keton)	90-94-8	0.01 mg/kg
Benzophenone	119-61-9	0. 0.1 mg/kg
2,4-Dihydroxybenzophenone	131-56-6	0.01 mg/kg
2-Methylbenzophenone	131-58-8	0.01 mg/kg
4-Methylbenzophenone	134-84-9	0.01 mg/kg
Methyl-2-benzoylbenzoate (MBB)	606-28-0	0.01 mg/kg
4,4'-Dihydroxybenzophenone	611-99-4	0.01 mg/kg
1-Hydroxycyclohexyl-1-phenyl ketone (Irgacure 184)	947-19-3	0.01 mg/kg
4-Phenyl benzophenone	2128-93-0	0.01 mg/kg
2-Isopropylthioxanthone (2-ITX)	5495-84-1	0.01 mg/kg
2-Hydroxy-2-methylpropiophenone (Photocure 50)	7473-98-5	0.01 mg/kg
4-Dimethylaminobenzoic acid ethyl ester (Firstcure EDAB)	10287-53-3	0.01 mg/kg
2-Ethylhexyl 4-(dimethylamino)benzoate (Quantacure EHA)	21245-02-3	0.01 mg/kg
2,2-Dimethoxy 2-phenyl acetophenone (Irgacure 651)	24650-42-8	0.01 mg/kg
Benzoic acid, 4-(dimethylamino)-, 2-butoxyethyl ester (Speedcure BEDB)	67362-76-9	0.01 mg/kg
2-Methyl-4'-(methylthio)-2-morpholinopropiophenone (Irgacure 907)	71868-10-5	0.01 mg/kg
Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide (Photocure TPO/ Lucerin TPO)	75980-60-8	0.01 mg/kg
2,4-Diethyl-9H-thioxanthen-9-one (Photocure DEXT)	82799-44-8	0.01 mg/kg
Ethyl (2,4,6-trimethylbenzoyl) phenylphosphinate (Lucirin TPO-L)	84434-11-7	0.01 mg/kg
2-Hydroxy-4'-(2-hydroxyethoxy)-2-methylpropiophenone (Irgacure 2959)	106797-53-9	0.01 mg/kg
2-Benzyl-2-(dimethylamino)-4'-morpholinobutyrophenone (Irgacure 369)	119313-12-1	0.01 mg/kg
1-Chlor-4-propoxythioxanthone (Speedcure CPTX)	142770-42-1	0.01 mg/kg
UV-Acrylatmonomers		
Tetraethylene glycol dimethacrylate	109-17-1	0.01 mg/kg
Triethylene glycol diacrylate (TriEGDA)	1680-21-3	0.01 mg/kg
2-(Dimethylamino)ethyl methacrylate	2867-47-2	0.01 mg/kg
Pentaerythritol triacrylate (PETA)	3524-68-3	0.01 mg/kg
Di(ethylene glycol) diacrylate (DEGDA)	4074-88-8	0.01 mg/kg
Pentaerythritol tetraacrylate (PETetraA))	4986-89-4	0.01 mg/kg
Trimethylolpropane triacrylate (TMPTriA	15625-89-5	0.01 mg/kg
Ethoxylated trimethylolpropane triacrylate (eoTMPTA)	28961-43-5	0.01 mg/kg
Dipentaerythritol hexaacrylate (DPEHA)	29570-58-9	0.01 mg/kg
Tri(propylene glycol) diacrylate (TPGDA)	42978-66-5	0.01 mg/kg
Pentaerythritol [5 EO] tetraacrylate (PPTTA B)	51728-26-8	0.01 mg/kg
Glycerol propoxylat (1 PO/OH) triacrylate (GPTA)	52408-84-1	0.01 mg/kg
Bisphenol A Epoxy diacrylate	55818-57-0	0.01 mg/kg
Dipropylene Glycerol Diacrylate (DPGDA)	57472-68-1	0.01 mg/kg
Dipentaerythritol pentaacrylate (DPEPA)	60506-81-2	0.01 mg/kg

Component	CAS No.	Detection limit [mg/kg]
Neopentyl glycol propoxylate (1 PO/OH) diacrylate (POMPGDA)	84170-74-1	0.01 mg/kg
Di(trimethylolpropane) tetraacrylate (DiTMPTetraA)	94108-97-1	001 mg/kg
Pentaerythritol, ethoxylated, propoxylated, acrylated (PPTTA A)	144086-02-2	0.01 mg/kg
Crosslinking agents from Epoxy resins		
BADGE, Bisphenol A diglycidyl ether	1675-54-3	0.01 mg/kg
BADGE.2H2O, Bisphenol A bis(2,3-dihydroxypropyl) ether	5581-32-8	0.01 mg/kg
BADGE.H2O, Bisphenol A (2,3-dihydroxypropyl) glycidyl ether	76002-91-0	0.01 mg/kg
BADGE.HCL, Bisphenol A (3-chloro-2-hydroxypropyl)	13836-48-1	0.01 mg/kg
glycidyl ether		
Badge 2HCl	4809-35-2	0.01 mg/kg
Badge HCl H2O	227947-06-0	0.01 mg/kg
BFDGE, Bisphenol F diglycidyl ether	06-03-2095	0.01 mg/kg
Noge	158163-01-0	0.01 mg/kg
Plasticizer		
Dicyclohexyl phthalate	84-61-7	0.01 mg/kg
Diethyl phthalate	84-66-2	0.01 mg/kg
Diisobutyl phthalate	84-69-5	0.01 mg/kg
Dibutyl phthalate	84-74-2	0.01 mg/kg
Dihexyl phthalate	84-75-3	0.01 mg/kg
Benzyl butyl phthalate	85-68-7	0.01 mg/kg
Diisopropyl phthalate	605-45-8	0.01 mg/kg
Bis(2-ethylhexyl) phthalate	117-81-7	0.01 mg/kg
Di-n-octyl phthalate	117-84-0	0. 01 mg/kg
Di-n-pentyl phthalate	131-18-0	0.01 mg/kg
Di-n-propyl phthalate	131-16-8	0.01 mg/kg
Diheptyl phthalate	3648-21-3	0.01 mg/kg
Diisooctyl phthalate	27554-26-3	0.01 mg/kg
Dimethyl sebaccate	106-79-6	0.01 mg/kg
Dibutyl sebaccate	109-43-3	0.01 mg/kg
Diethyl sebaccate	110-40-7	0.01 mg/kg
Triethyl citrate	77-93-0	0.01 mg/kg
Tributyl citrate	77-94-1	0.01 mg/kg
Dibutyl adipate	105-99-7	0.01 mg/kg
Diisobutyl adipate	141-04-8	0.01 mg/kg
Diethyl adipate	141-28-6	0.01 mg/kg
Tributyl O-acetylcitrate	77-90-7	0.01 mg/kg
Tris(2-chloroethyl) phosphate	115-96-8	0.01 mg/kg
N-Ethyl-p-toluenesulfonamide	80-39-7	0.01 mg/kg
Miscellaneous		
Salicylic acid	69-72-7	0.01 mg/kg
Anthranilamide	88-68-6	0.01 mg/kg
Propyl 4-hydroxybenzoate	94-13-3	0.01 mg/kg

Component	CAS No.	Detection limit [mg/kg]
4,4'-Thiobis(6-tert-Butyl-m-cresol)	96-69-5	0.01 mg/kg
Dichlorophen	97-23-4	0.01 mg/kg
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	102-60-3	0.01 mg/kg
Triethanolamine	102-71-6	0.01 mg/kg
2,2'-Methylenebis(6-tert-butyl-4-methylphenol)	119-47-1	0.01 mg/kg
Ethyl 4-hydroxybenzoate	120-47-8	0.01 mg/kg
Azelaic acid	123-99-9	0.01 mg/kg
2-Hydroxy-4-methoxy benzophenone	131-57-7	0.01 mg/kg
Benzoic acid, p-(dimethylamino)	619-84-1	0.01 mg/kg
2,4,6-trimethylbenzophenone	954-16-5	0.01 mg/kg
2-Ethylhexyl diphenyl phosphate	1241-94-7	0.01 mg/kg
Tricresyl phosphate	1330-78-5	0.01 mg/kg
2,2-Diethoxy acetophenone	6175-45-7	0.01 mg/kg

Appendix 6: Metals examined by ICP/MS screening

TABLE 42 Metals examined by ICP/MS screening and their associated detection limit expressed as [mg] metal per [kg] product simulant (3 % acetic acid). Results are expressed as [mg] analyte per [kg] product simulant.

Metal	Detection limit [mg/kg]	Metal	Detection limit [mg/kg]
Lithium	0.007	Tin	0.08
Beryllium	0.03	Antimony	0.08
Boron	0.3	Tellurium	0.08
Sodium	0.08	Cesium	0.08
Magnesium	0.08	Barium	0.08
Aluminum	0.3	Lanthanum	0.08
Potassium	0.007	Cerium	0.08
Calcium	0.007	Praseodymium	0.08
Scandium	0.007	Neodymium	0.08
Titanium	0.007	Samarium	0.08
Vanadium	0.04	Europium	0.08
Chromium	0.007	Gadolinium	0.08
Manganese	0.007	Terbium	0.08
Iron	0.007	Dysprosium	0.08
Cobalt	0.02	Holmium	0.08
Nickel	0.007	Erbium	0.08
Copper	0.007	Thulium	0.08
Zinc	0.08	Ytterbium	0.08
Gallium	0.04	Lutetium	0.02
Arsenic	0.007	Hafnium	0.08
Selenium	0.007	Tantalum	0.08
Rubidium	0.007	Tungsten	0.08
Strontium	0.007	Osmium	0.08
Yttrium	0.007	Iridium	0.007
Zirconium	0.007	Platin	0.007
Niobium	0.007	Gold	0.007
Molybdenum	0.007	Mercury	0.007
Ruthenium	0.007	Thallium	0.08
Palladium	0.007	Lead	0.007
Silver	0.007	Bismuth	0.007
Cadmium	0.007	Thorium	0.007
Indium	0.007	Uranium	0.007

Appendix 7: Data for calculation of MoS values

In the following, data for calculating the Margin of Safety (MoS) of the six selected substances/groups of substances in three of the analyzed PCR plastic samples are summarized.

TABLE 43 Computation of MoS for PCR-sample no.1.1

Name of substance	CAS No.	Measured conc. (mg/kg)	Absorption via skin (fraction) P	TDI (DNEL) (mg/kg bw/day)	SED (mg/kg bw/day) Baby body lotion	SED (mg/kg bw/day) Shampoo	MoS Baby body lotion	MoS Shampoo
Benzophenone	119-61-9	1.2	0.7	0.03	0.00027	4.08E-06	110	7349
Dibutyl phthalate (DBP)	84-74-2	0.098	0.1	0.0067	3.1703E-06	4.7628E-08	2113	140674
Diethylhexyl phthalate (DEHP)	117-81-7	5.6	0.05	0.05	0.00009	1.3608E-06	552	36743
SUM DEHP, DBP (x5 =0.49)	-	6.09	0.1	0.05	0.00020	2.95974E-06	254	16893
Tris-(2,4-di-t-butylphenyl)-phosphite	31570-04-4	110	1	0.6	0.03559	0.0005346	17	1122
2,6-bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	0.33	0.134	0.25	1.43E-05	2.14E-07	17476	1163282

TABLE 44 Calculation of MoS for PCR plastic sample no. 5.3

Name of substance	CAS No.	Measured conc. (mg/kg)	Absorption via skin (fraction) P	TDI (DNEL) (mg/kg bw/day)	SED (mg/kg bw/day) Baby body lotion	SED (mg/kg bw/day) Shampoo	MoS Baby body lotion	MoS Shampoo
2,4-di-tert-butylphenol	96-76-4	6.5	1	0.007	0.00210	0.00003159	3	222
2,6-bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	5.9	0.134	0.25	0.00026	3.84232E-06	977	65065
Dibutyl phthalate (DBP)	84-74-2	4.5	0.1	0.0067	0.00015	0.000002187	46	3064
Diethylhexyl phthalate (DEHP)	117-81-7	10	0.05	0.05	0.00016	0.00000243	309	20576
SUM DEHP, DBP(x5=22,5)	-	32.5	0.1	0.05	0.00105	0.000015795	48	3166

TABLE 45 Calculation of MoS for PCR plastic sample no. 5.4

Name of substance	CAS No.	Measured conc. (mg/kg)	Absorption via skin (fraction) P	TDI (DNEL) (mg/kg bw/day)	SED (mg/kg bw/day) Baby body lotion	SED (mg/kg bw/day) Shampoo	MoS Baby body lotion	MoS Shampoo
AI		0.6						
Benzophenone	119-61-9	0.58	0.7	0.03	0.00013	1.97316E-06	228	15204
Dibutyl phthalate (DBP)	84-74-2	1.8	0.1	0.0067	0.000058	8.74E-07	115	7659
2,4-di-tert-butylphenol	96-76-4	4.6	1	0.007	0.00149	0.000022356	5	313
2,6-bis(1,1-dimethyl)-4-methylphenol (BHT)	128-37-0	2.4	0.134	0.25	0.00010	1.56298E-06	2403	159951
Tris-(2,4-di-t-butylphenyl) phosphite	31570-04-4	3.8	1	0.6	0.00122	0.000018	488	32489

Initial safety assessment of recycled plastic for packaging of cosmetic products

This report describes the results of the project on initial safety assessment of recycled plastic for packaging of cosmetic products such as shampoo, body lotion or liquid soap. The recycled plastic in focus is post-consumer recycled plastic (PCR plastic) obtained from relevant stakeholders in the Danish industry. Initially, the PCR material samples with accompanying documentation were collected and assessed, and then specific samples were selected for analysis and safety assessment. An analysis program for migration studies followed by broader screenings of ingredient substances and substance-specific analyses were combined and carried out to generate knowledge on the chemistry in PCR materials. Finally, a safety assessment was performed for specific chemical substances in selected PCR materials based on the results of chemical analysis.

The project was carried out during the period from August to December 2020 for Danish Environmental Protection Agency by Danish Technological Institute with DHI as subcontractor.

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