

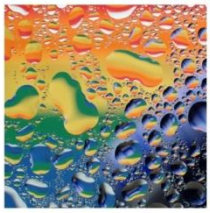

Risks to drinking water from Personal Care Products and Domestic Cleaning Products

WRc Ref: DWI9879.03
June 2014

Risks to drinking water from Personal Care Products and Domestic Cleaning Products

Report No.:	DWI9879.03
Date:	June 2014
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Summary

i Reasons

Personal care products (PCPs) and domestic cleaning products (DCPs) are a diverse range of products that contain vast numbers of different chemicals. These chemicals may have the potential to reach drinking water supplies via release into the environment through typical use and entry to sewerage and subsequent treatment. Published studies from other countries on the occurrence of substances from PCPs and DCPs, demonstrate that trace amounts of these constituents can reach drinking water. A similar situation may be expected, in England and Wales, however, no information is currently available.

ii Objectives

This study presents an investigation into the potential for ingredients used in personal care products (PCPs) and domestic cleaning products (DCPs) to be present in drinking water. An assessment was also made as to the potential for people to be exposed to these ingredients at higher concentrations from drinking water and bathing than would be anticipated through the intended use of PCPs and DCPs.

iii Benefits

This project has collated available data on 692 chemicals that are commonly used in PCPs and DCPs. These chemicals were screened to develop a shortlist of chemicals that were identified as having a higher potential to occur in drinking water. These 'priority chemicals' were then assessed to compare their predicted exposure via drinking water and bathing to use from typical use. This provides a focus for further work that may be required to assess the potential for PCPs and DCPs to occur in drinking water in the UK.

iv Conclusions

Approximately 690 chemicals were assessed and thirty-three of these chemicals were identified during the data collation and prioritisation exercise as having a high potential for reaching drinking water supplies. The prioritisation was based on parameters such as the physico-chemical properties of the chemicals, the annual consumption tonnages of each chemical and whether studies were available in the public literature reporting their prior detection in drinking water. The potential concentration of these chemicals in drinking water was then modelled. The precautionary estimated exposure to these chemicals via drinking water and bathing was compared to the estimates of exposure to these same chemicals through their intended use.

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Out of the thirty-three prioritised chemicals, the models indicated that exposure via drinking water and bathing was significantly lower for nineteen chemicals than would be anticipated through their intended use.

However, ten of the thirty-three prioritised chemicals were predicted to produce levels of maximum exposure through drinking water and bathing close to or greater than would be anticipated through their intended use. Data were lacking for the four remaining chemicals, and therefore a comparison of exposure via these routes could not be conducted.

v Suggestions

Targeted monitoring for the chemicals that appear to have the greatest potential to occur in drinking water could be used to verify the model and inform whether these chemicals are an issue in drinking water in the UK.

Further data collation and development of a relevant exposure model from typical use of the four chemicals that do not have authoritative exposure assessments would enable assessment of these chemicals.

The developed predictive model is precautionary and additional data on removal efficiencies in waste water treatment and drinking water treatment could help refine the model.

Collection and assessment of data on the toxicological properties of those chemicals that have been identified as having the highest potential to reach drinking water in significant concentrations would also inform whether these chemicals are of concern in drinking water supplies.

vi Résumé of Contents

This document describes the approaches used to identify and prioritise the PCPs and DCPs, the development of an exposure assessment process to screen and model the potential exposure to chemicals present in PCPs and DCPs via drinking water and bathing, and a comparison of that exposure with anticipated exposure resulting from the typical uses of PCPs and DCPs.

Stage 1: Data collation and screening of 692 chemicals to devise a list of thirty-three priority chemicals.

Stage 2: Modelling of potential concentrations in drinking waters and comparison with literature data.

Stage 3: Exposure assessment and comparison of potential exposures via drinking water and bathing with exposure from intended use of the PCPs and DCPs.

1. Introduction

The aim of this research project was to understand any potential exposure to personal care products (PCPs) and domestic cleaning products (DCPs) present in drinking water in England and Wales and to compare such exposure with that following intended use of these products.

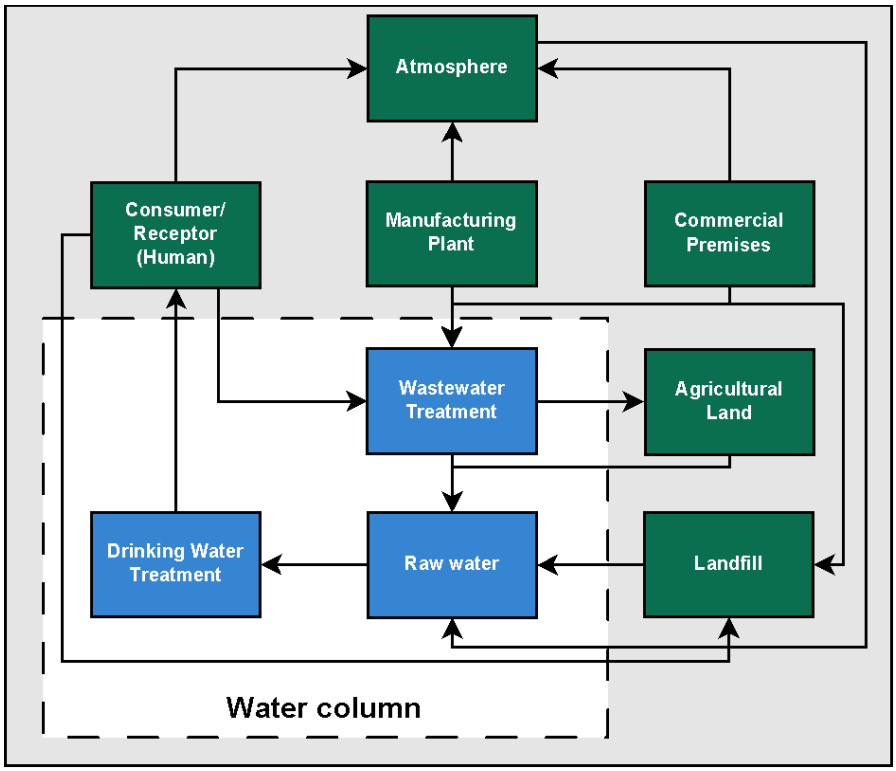
Personal Care Products are a diverse range of products (from baby products to hair colorants), which include fragrances, hair care products, lotions and cosmetics. Domestic cleaning products (DCPs) include washing powders and liquids, fabric conditioners, bar soaps, hand and machine dishwashing products, household disinfectants, and polishes and specialist cleaners for use in kitchens and bathrooms. The typical use of these products will result in release of these substances to the drain, their entry into sewers and wastewater treatment plants. If wastewater treatment processes do not remove all of the substances, they may enter water bodies in the environment and, potentially, enter drinking water supplies. Published studies from other countries on the environmental occurrence of substances from PCPs and DCPs, demonstrate that trace amounts can reach drinking water. Although a similar situation may be expected, in England and Wales, no information is currently available.

1.1 Routes to water

To develop the model to predict the potential concentration of each chemical in drinking water the route these chemicals take to reach the water supply must be assessed. A broad assessment of each product type has been conducted which aims to indicate the main route of these chemicals to the drinking water supply.

Figure 1.1 provides conceptual pathways by which PCP and DCPs may potentially reach the consumer.

Figure 1.1 Environmental exposure pathways



1.1.1 Personal Care Products

There are many different types of PCP and DCP with different use patterns and therefore different pathways to the human receptor. Therefore levels of duration and exposure can vary significantly as can their routes to water.

Leave-on products

'Leave-on' products include cosmetics, moisturisers, leave in hair conditioners fragrances, body sprays and deodorants. On application of these products to the skin or hair, it is expected that excess product may be rinsed off hands or applicators, resulting in discharge into the sewerage system; however, some may volatilise to the atmosphere, especially fragrances, or be deposited on floors or surfaces (such as sinks and basins). Some of the ingredients in the product may be absorbed through the skin and subsequently undergo metabolism and excretion. The amount absorbed will depend on the type of product applied, it is expected that moisturisers, which are designed to absorb into the skin, will be absorbed more rapidly than eye shadows or foundation, which is designed to sit on the surface. However, it is also worth noting that the combination of chemicals present in cosmetics may alter the rate of absorption of other chemicals. For example, components of cosmetics which may have low potential for dermal absorption when applied on their own may be absorbed more readily in the presence of the other components of cosmetics.

During the day, these ‘leave–on’ products may rub off onto clothing, surfaces or other people through personal contact. Products like cosmetics will be washed off at the end of the day, resulting in release to the sewerage system, although some will be wiped off using disposable wipes or cotton wool and disposed of to the municipal solid waste stream. Products on clothing will be washed off during laundering and enter the sewerage system. Products that end up on the floors or surfaces are usually either washed off during cleaning and end up in the sewerage system or are swept up or vacuumed up before being placed in the municipal solid waste stream. Left over products may be either disposed of to the municipal solid waste stream or washed down into the sewerage system.

Products such as hair dyes can be considered to be both ‘leave-on’ and ‘rinse-off’ products. The colour that stays on the hair is either permanent (will not be removed from the hair) or semi-permanent (will gradually wash out of the hair over a specified period). The vehicle for delivering the dye to the hair is usually a mixture of chemicals that are rinsed off straight to the sewerage system.

Rinse-off products

‘Rinse–off’ products include shampoos, soaps, shower gels and shaving gels. Application to the hair or skin is normally for a limited time before they are washed off and disposed directly into the sewerage system. As with leave-on products, a small amount may be absorbed or residue may remain on skin or hair for a longer duration, and like ‘leave-on’ products, will be subject to deposition on clothes, surfaces or other people. However, the amount of product left on the hair or skin will be much lower for ‘rinse-off’ products than for ‘leave-on’ products. Some of the products may volatilise or be deposited on floors or other surfaces which will either be washed to sewerage or vacuumed. Volatilised products are likely to be very small in quantity. The majority of rinse-off products will go straight to the sewerage system through typical use. Left over products are most likely to either disposed of to the municipal solid waste stream or washed down into the sewerage system.

Oral care products

Oral care products include toothpastes, gels and mouthwashes. Exposure to these products is different to that of ‘leave-on’ or ‘rinse-off’ products, as oral care products are intentionally applied to the inside of the mouth, which increases the chance that the product will be ingested or absorbed through the inside of the mouth. Oral products are largely designed to be rinsed out of the mouth, resulting in their release to the sewerage system. However, some remaining product, for example, the remaining material in a tube of toothpaste may enter the municipal solid waste stream. Products such as dental floss are designed to be removed from the mouth and placed into the waste.

1.1.2 Domestic cleaning products

Laundry care/ dish care

Laundry care and dish care products include dishwasher tablets/powders, washing up liquids, and laundry powders, liquids and softeners or tablets. The majority of these products are 'rinse-off' products that are diluted in water and used to wash clothes or dishes. Whether in a dishwasher or a clothes washer, the majority of the product will be discharged into the sewerage system. It is likely that some product will remain on the clothes or dishes after washing. Some of this residue may volatilise during heat drying. However, residues left on the dishes or clothes may results in contact directly with the skin, or migration to food or drink that will be ingested. Therefore, there is potential for some absorption of these products to occur.

Surface cleaning

Surface care products include hard surface cleaners such as kitchen and bathroom spray cleaners, gel and abrasive cleaners, furniture polishes and waxes. Some of these products are rinse-off products that are washed or wiped off after cleaning and rinsed into the sewerage system. Exposure will initially be from contact with the product through their intended use, although some of these products are designed to leave a residue on the hard surface such as furniture polishes and waxes, and therefore exposure may occur through contact with the hard surface sometime after cleaning. Exposure may also occur via inhalation of the spray. It is assumed that the majority of the product will be washed to the sewerage system either directly through typical use or from laundering or rinsing of cloths that may be used to apply the cleaner.

Air care

Air care includes air fresheners and fragrances. Products that are sprayed into the air will either degrade in the atmosphere or eventually be deposited on surfaces or carpets and washed off or vacuumed up. Products such as air freshening gels are less likely to end up on surfaces but may end up in the solid municipal waste stream. The main route of exposure to these products will be through inhalation, although deposited product may also be absorbed dermally.

Floor care

Hard surface floor care like hard surface cleaners are most likely to end up being washed into the sewerage system after rinsing. Soft floor cleaners such as carpet shampoos will most likely end up in the sewerage system as they are applied then removed again and disposed to sewer. Powder cleaners, however, are normally vacuumed from the carpet and disposed of to the solid municipal waste stream. The largest exposure will be through using the floor cleaners and residues may come into contact with skin, mostly through the bottom of the feet. Young children may have more dermal contact with residues on any floor surface.

1.1.3 Exposure to these products from via ingestion of food from agriculture

There is a possibility that people could be exposed to these products via the food that they eat. Any compounds that are present in the soil or water though contamination by sewage sludge or river water could potentially reach people via the food that is grown on the land. It is thought that this exposure route would be minimal and significantly less than the potential uptake via normal use of the PCPs or DCPs or via drinking water and bathing. As such this has not been assessed as part of this project.

1.2 Summary

The majority of the PCPs and DCPs used in the domestic environment will go to the sewerage system with small amounts being released to air or remaining on surfaces as residues. There may be significant input to municipal waste but it is not possible to identify how much of these chemicals end up in the solid waste stream. Following wastewater treatment these chemicals may enter the environment via the effluent and enter drinking water treatments works after abstraction from water courses. There is also the possibility that people could be exposed via drinking water.

2. Risk Assessment Approach

To assess the risks of PCPs and DCPs entering UK water supplies a staged approach has been devised.

Stage 1: A literature search was conducted to formulate a list of potential chemicals that might arise from the use of various PCPs and DCPs in the domestic environment. As much data for each chemical was collated from literature that covers the following parameters:

- Type of product in the UK
- Tonnage used in the UK
- Physico-chemical parameters (e.g. volatility, log Kow, solubility)
- Occurrence in influent, sewage, surface water/groundwater and drinking water
- Removal during wastewater and drinking water treatment
- Toxicity

A prioritisation process was devised using this data to identify the chemicals that are most likely to occur in UK drinking water supplies.

Stage 2: The potential routes for these prioritised chemicals to reach drinking water were examined and assessed. A simple, conservative model (Section 4.1) was developed to derive potential concentrations of these chemicals in drinking water supplies. These concentrations were then compared with real occurrence data to validate the results of the model. These chemicals were then ranked to highlight those with the potential for the highest concentrations to occur in drinking water.

Stage 3: Consumer exposure estimates for typical use of these chemicals were sought from literature and authoritative risk assessments. The Systemic Exposure Dose (SED) to these chemicals through intended use was compared to the estimated exposure from drinking water and bathing. Any chemical which has an estimated exposure through drinking water and bathing that is less than the SED through intended use of the DCPs or PCPs was ranked as being of very low risk to drinking water supplies. The remaining chemicals were highlighted as potential chemicals as potentially requiring further consideration.

3. Stage 1: Literature Search and Prioritisation

Stage 1 of the project was designed to develop a comprehensive list of chemicals used as ingredients in Personal Care Products (PCPs) and Domestic Cleaning Products (DCPs). These chemicals were then assessed for their potential to reach drinking water in significant amounts. This identified a short list of chemicals that would be taken through to model their potential concentrations in drinking water.

3.1 Data search

3.1.1 Data requirements

The largest component of this project was the collation of data. A search structure was developed in order to collect as much relevant data as possible on the potential ingredients found in PCPs and DCPs considering the following categories.

Products

- Product type: personal care products (PCPs):
  - baby products,
  - bath products,
  - make-up products,
  - hair care products,
  - hair colorants,
  - nail products,
  - oral care products,
  - personal cleanliness products,
  - shaving products,
  - sunscreen and suntan products,
  - skin care products.
- Product type: domestic cleaning products (DCPs):
  - washing powders and liquids,
  - fabric conditioners,
  - laundry additives,
  - bar soaps,
  - hand and machine dish wash,
  - household disinfectants,
  - polishes and specialist cleaners for use in kitchens and bathrooms.

Constituents

- Common constituents including, lipophilic care components and emulsifiers, fruit acids and solvent alcohols, polymers, preservatives, dyestuffs, perfume oils and propellants.

Usage and tonnage data

- Usage of each constituent in PCPs and DCPs.
- Tonnage used in the UK.

Typical exposure

- Regulatory control (Biocidal Products Directive, REACH or Cosmetics Regulation).
- Use/exposure route (oral, skin application, bathing, hard surface cleaning, machine washing and dishwashing).
- Typical daily human exposure from application or use of PCPs or DCPs.

Environmental Fate and behaviour

- Physico-chemical properties.
- Data on photolysis, hydrolysis and biodegradation.
- Wastewater and drinking water treatment/removal.
- Occurrence (raw and treated drinking water).

3.1.2 Search framework

A reproducible and robust searching framework was established to locate data on the substances used in PCPs and DCPs. A number of sources of information have been used to collate relevant data (See Table 3.1 for a full list).

Table 3.1 Data gathered during collation exercise

Chemical identification	Physico chemical properties	Usage Tonnage information	Routes, water identity	Toxicity
Main category/type of PCP or DCP	Molecular weight (g mol^{-1})	Usage/Tonnage data	Occurrence Water supply score	Toxicity information
Chemical name (common)	Melting point (°C)	Used in DCPs/PCPs tonnes/year	Occurrence raw water score	CLP classification Harmonised/not harmonised
CAS number	Boiling point (°C)	Used/sold total tonnes/year	Occurrence waste water score	CLP Acute toxicity
	Water solubility (mg/l)	Manufactured tonnes/year	Routes, water identity	CLP Mutagenic
	Partition coefficient - Log Kow		Removal from waste water	CLP Carcinogenic
	Vapour pressure (hPa)		Removal from drinking water	CLP Reproductive toxicity
	pKa – acid dissocation constant			CLP Sensitising
	Henrys law constant (atm m^3/mol)			CLP Irritant
	Biodegradation			CLP Specific Target Organ Toxicity
	Hydrolysis			Typical (estimated) exposure concentrations
	Photolysis			

The first task was to produce a comprehensive list of the potential chemical substances that could be present in PCPs and DCPs. Information on this aspect was sourced initially from trade associations which listed common ingredients used in different types of PCP or DCP product. All of the common ingredients listed by these trade associations for the various PCP or DCP types were listed replications were omitted and this formed the initial chemical list. The following trade associations were interrogated to form the initial chemical list:

- Cleanright – European industry supported website contains a list of ingredients used in DCPs;
- Cosmetics Info – database of ingredients contained in cosmetics by category;
- Cosmetics Europe – The Personal Care Association (formerly COLIPA);

- The Cosmetic, Toiletries and Perfumery Association;
- The Personal Care Products Council (US);
- The UK Cleaning Products Association.

This initial list, however, omitted some of the chemical ingredient types that have been identified in the literature (KIWA, 2004, Reif *et al.,* 2011, Janna *et al.,* 2011, Kanda *et al.,* 2003, Kasprzyk-Hordern *et al., 2009,* and Stuart *et al.,* 2012) as substances considered as having potential to reach drinking water. Information from this data search was used to supplement the list of chemicals collated from the aforementioned trade associations. This resulted in a list of ~600 chemicals. These specific chemical types included: Musks (nitro musks – musk xylene, musk ketone; polycyclic musks – tonalide, galaxolide, celestolide; macrocyclic musks – ambrettolide, cyclopentadecenolide) (Chemical lists developed using these references: Boots, 2012, The HERA Project, 2012, CosIng, 2012, The Good Scents Company, 2012);

- Parabens (butylparaben, methylparaben, propylparaben, ethylparaben) (Chemical list developed from CosIng, 2012);
- Phthalates (di(ethylhexyl)phthalate (DEHP), di-iso-nonylphthalate (DINP), di-iso-decylphthalate (DIDP), dimethylphthalate (DMP), diethylphthalate (DEP), dibutylphthalate (DBP)) (Chemical list from CosIng, 2012);
- Biocides (Triclosan - Microban®);
- Insect repellents (N,N-diethyl-meta-toluamide (DEET)) (Chemical list from HPA, 2012);
- UV filters/sunscreens (benzophenones) (Chemical list from CosIng, 2012);
- Dishwasher cleaning products (benzotriazoles, tolyltriazole) (Chemical list from Janna *et al.,* 2011); and
- Skin protectants (siloxanes).

Risk assessments specific to PCP and DCP ingredients, were then interrogated to identify any chemicals that were no included in the list of 600 chemicals but were assessed by these other projects and to gather relevant information that was used in the prioritisation and subsequent modelling process.

These sources included:

- the Human and Environmental Risk Assessment (HERA) project on Ingredients of European Household Cleaning Products; and
- the Opinions from the European Scientific Committee on Consumer Products.

The HERA project contained data on substances used in household detergent and cleaning products, consumer use, endpoints of concern for consumer exposures and environmental compartments of relevance.

The list that was produced contained 692 chemicals (See Appendix B). The chemical names and CAS numbers were then used as search terms to gather the required data for the prioritisation and modelling stages of the project.

- Authoritative risk assessments were then sought for each of the 692 chemicals and the relevant data collated. These sources contained data on uses, occurrence and human health risk assessments. The following authoritative risk assessment databases were searched and the data collated: The Cosmetics Ingredient Review:
- EU risk assessments under the Existing Substances Regulation;
- European Union Risk Assessment Reports (EU RAR);
- the OECD High Production Volume (HPV) chemicals programme;
- the International Council of Chemical Associations (ICCA) HPV initiative;
- the International Programme on Chemical Safety (IPCS) (WHO) Concise International Chemical Assessment Documents (CICADs).

The following sources were then investigated to address any data gaps:

- International Uniform Chemical Information Database (IUCLID), Hazardous Substances Databank (HSDB), United States Environmental Protection Agency (US EPA). These were considered to be sound data sources as they are governmental/regulatory data sources; however they may not be peer reviewed sources and were considered to be secondary to the authoritative risk assessments. These sources were used to address gaps in the physic-chemical and environmental fate and behaviour data.
- REACH dossiers for specific chemicals registered to date, available from the European Chemicals Agency (ECHA) website. The data in these dossiers were used with caution as the data in the majority of them has not been verified.

- The Classification Labelling and Packaging (CLP) Database which contains the harmonised and non-harmonised self-classifications under the Classification Labelling and Packaging (CLP) Regulations (EC no. 1272/2008), available from the European Chemicals Agency (ECHA) website. These classifications have been used to indicate whether a chemical has potential human health effects. It was noted that non-harmonised classifications, unlike harmonised classifications, have not been peer reviewed and the conclusions have not been verified and agreed. Despite this these classifications have been used to give an indication of whether the chemical might exhibit a potential toxic effect. This was used only to offer a screen for such a large number of chemicals and detailed analysis of the potential toxicity of these chemicals has not been undertaken.

- UK Office for National Statistics. Data were available on the sale, import and export tonnages of chemicals and chemical products in the UK (however, some data points are suppressed as they are considered to be commercially confidential).

- EUROSTAT holds data on manufactured chemicals by kg volume in the UK.

  Note: all the data sources used in this study are listed in Appendix A of this report.

3.1.3 Data collation

The literature search identified 692 chemicals that are commonly used by members of relevant trade associations, identified as requiring authoritative risk assessments by governmental organisations or interest groups, or have been identified in the regulations as being part of a specific group of chemicals of interest. This list is not exhaustive, but gave a good basis for determining potential chemicals that warranted further investigation in the subsequent exposure assessment (See Appendix B).

3.1.4 Data Gaps

As much general data as practicable for such a large number of chemicals have been gathered from the sources listed in this section. However there were still a large number of gaps in the data, including chemicals for which no data could be located (including a CAS number for identification) and chemicals that have limited physico-chemical data and/or no human health assessments or prior risk assessments.

The largest data gap identified relates to usage and market trend data for ingredients used in PCPs and DCPs - meaningful usage data for such a large, diverse list of ingredients are inherently difficult to obtain. Studies conducted under the HERA project provided some usage data for ingredients in domestic cleaning products as part of an exercise modelling predicted environmental concentrations. The HERA project did not include usage data for chemicals used in PCPs. Occasionally usage data were located in other studies but the scale of the data was variable and included global, US and European usage figures.

The UK Office of National Statistics had “net supply” data on only a few chemicals and did not include a breakdown on which industrial sectors used this supply. The chemicals with REACH dossiers could be placed in broad ranges of tonnages that are manufactured or imported into Europe, but again, this did not indicate in which market sector these chemicals are used or what proportion is used in PCPs or DCPs. As such WRc approached Euromonitor who gather market data including trends and market sector use within the UK. It was still not possible to obtain market data for all of the chemicals but the data provided by Euromonitor were considered the most detailed and up to date (2012 data) that could be obtained for the UK.

3.1.5 Summary

A large list of relevant chemicals (692 listed in Appendix B) was developed using information from trade associations, governmental organisations and specialist interest groups. Once these chemicals were identified, a range of data was sought on the properties of these chemicals. This information was collated and gaps within this data were located.

3.2 Prioritisation

3.2.1 Review of Relevant Criteria

An example of typical criteria for prioritising chemicals of concern that has been developed by HERA is presented below, this approach is similar to approaches used by scientific bodies such as the European Scientific Committee on Consumer Products. This provides insight into aspects that are currently used to identify priority chemicals of concern and ensures that these aspects are captured in a systematic way. This approach was used as a starting point for the establishment of the criteria to identify PCPs and DCPs for this study.

The existing criteria are part of a risk based approach and incorporate:

- Hazard assessment.
- Exposure assessment.
- These are subsequently combined to provide a number for ranking according to the risk that they pose. The Human and Environmental Risk Assessment on Ingredients of Household Cleaning Products (HERA) uses the following criteria to prioritise the chemicals they examine (HERA, 2002).
- **High tonnage chemicals** (This is especially relevant for an industry characterised by chemicals used in very large quantities sold directly to consumers).
- **Main or sole use in detergents and cleaning products** (This ensures that the targeted risk assessment covers the majority of uses in a manner which is as defensible as possible.)

- **Initially, at least one substance per important function, e.g. surfactants, builders, bleaches, etc.** (In this way HERA ensures as representative a sample as possible of substances used in the industry.)

- **Chemical selection covers a wide range of hazard profiles** (This allows coverage of a broad range of risk assessment situations and to demonstrate that HERA is not selecting only the 'easy' case.)

- **Chemicals on the EU Priority Lists are included.**

- **Complementarity with other programmes** e.g. the EU Existing Chemicals Programme, the ICCA HPV Initiative, and the OECD HPV Chemicals Programme.

- **Prioritisation of substances that HERA suspects of potential issues** (The intention is to point out the need for appropriate risk management decisions on these substances, if risk assessment demonstrates the need, and to provide information on which to base communications if no significant risk is identified under the exposure scenarios).

3.2.2 Prioritisation criteria

Due to the large number of chemicals in PCPs and DCPs currently in use it is not practical to assess the potential exposure of every chemical to humans. Therefore, a ranking exercise has been conducted to prioritise the relative importance of each chemical in each category to the UK population. A priority list of chemicals (or groups of chemicals) that could potentially reach drinking water has been selected to form the list of chemicals that will be studied further.

As part of this exercise, each chemical identified during the initial data search was scored according to criteria developed by WRc (See Table 3.2).

The criteria for "Known to have/may have adverse effects in humans" were based on entries in the Classification, Labelling and Packaging (CLP) database provided by the European Chemicals Agency (ECHA) (ECHA, 2013). Any entry that identified the compound to have adverse human health effects was given a score of three, despite whether they were harmonised or non-harmonised entries. The precautionary approach was taken that if a compound has been classed as having potential human health effects then priority should be given to that chemical, even if the evidence behind that classification is not accessible. Harmonised classifications that have no classification for human health effects were given a low score.

The criteria for solubility, volatility, sorption to organic matter were developed by WRc using guidance provided by ECHA (2012) and the US EPA (2012). A pragmatic decision for the development of the biodegradation, photolysis (degradation by light) and hydrolysis

(degradation when in contact with water) criteria was taken, as the data for these chemical properties were extremely varied in the level of detail provided. These criteria were developed based on the simple premise that any evidence that the compound is or is not degraded by organisms, light and water resulted in that compound being given high or low scores. Absence of degradation data was given a median score. Additional data such as rate of degradation (other than results from a "ready biodegradation" test) were not often reported in the literature and therefore difficult to assign criteria too.

The usage and manufacturing data criteria were also developed using expert judgement of the data as it was presented. The Euromonitor data used in the model in Section 4 was not included in this prioritisation process because most of the data was categorised into chemical groups and it would have been prohibitive to assign each of the 692 chemicals to a category. The data collated from literature included data from the UK, Europe and the rest of the world.

In some cases the data gathered for each chemical came from multiple sources, which reported the values in different ways using different units. The data were standardised as far as possible to establish if data from different literature sources reported significantly different for results for the same chemical. The original literature was reassessed for a few of the chemicals that had multiple data points that varied significantly and expert judgement was used to determine the most reliable result. Where multiple manufacturing/usage data points were found each tonnage was given an individual score then the maximum score for that chemical was used in the prioritisation. Where no data were available, a score of 2 was assigned. There were gaps in the data for approximately 73% of the endpoints. A higher combined score resulted in a greater prioritisation.

Table 3.2 Prioritisation criteria developed by WRc

Criteria	Importance	Parameter	Weighting (1 low: 3 high)
Known to have/may have adverse effects in humans	Chemicals which are known to cause, or are strongly suspected to cause adverse effects to human health are of high priority for weighting. It is important to quantify how much, if any, hazardous chemicals used in PCPs/domestic cleaning products are present in treated water in order to maintain the safety of drinking water for human consumption.	• Classification for human health hazards according to the CLP regulation harmonised classifications	3
		• Classification for human health hazards according to the CLP regulation non-harmonised classifications	3
		• Harmonised classification available but no human health effects listed	1

Criteria	Importance	Parameter	Weighting (1 low: 3 high)
		• No classification, but evidence from toxicology studies of potential for adverse effects	3
		• No classification and no additional data.	2
		• No classification, but evidence from toxicology studies that there are no human health effects	1
Not removed by wastewater treatment processes	Chemicals that have parameters indicating that they are likely to be readily and substantially removed by wastewater treatment processes are of low priority, as it is unlikely that they will be present in discharges to surface water in any substantial concentrations, and therefore will not be anticipated to occur in raw and or finished drinking water.	• Low log Kow (-ve to 3, unlikely to sorb to organic matter and likely to remain in water column)	3
		• Moderate log Kow (3 to 5, likely to moderately sorb to organic matter in the WwTW)	2
		• High log Kow (>5, very likely to sorb to organic matter in the WwTW)	1
		• High solubility (>1000 mg/l)	3
		• Moderate solubility (10-1000 mg/l)	2
		• Low solubility/negligible solubility (<10 mg/l)	1
		• Not biodegradable	3
		• Biodegradable	2
		• Readily/inherently biodegradable	1
Not easily removed by drinking water treatment processes (it is acknowledged that some drinking water has limited treatment, such as	Chemicals that have parameters indicating that they are likely to be removed by drinking water treatment processes are of low priority, as it is unlikely that they will be present in potable water.	• Low log Kow (-ve to 3, unlikely to sorb to organic matter and likely to remain in water column)	3
		• Moderate log Kow (3 to 5, likely to moderately sorb to organic matter)	2

Criteria	Importance	Parameter	Weighting (1 low: 3 high)
groundwater)		• High log Kow (>5, very likely to sorb to organic matter)	1
		• High solubility (>1000 mg/l)	3
		• Moderate solubility (10-1000 mg/l)	2
		• Low solubility/negligible solubility (<10 mg/l)	1
		• Not biodegradable	3
		• Biodegradable	2
		• Readily/inherently biodegradable	1
Level of abiotic degradation (hydrolysis and photolysis)	Chemicals that readily degrade by abiotic process are less likely to persist through wastewater treatment, drinking water treatment or in the environment.	• Stable to hydrolysis (does not degrade in contact water)	3
		• No data on hydrolysis	2
		• Hydrolyses (degrades in contact with water)	1
		• Stable to photolysis (does not degrade under natural light)	3
		• No data on photolysis	2
		• Photolyses (degrades under natural light)	1
		• Non-volatile (Henry's Law constant of $<1 \times 10^{-7}$)	3
		• Likely to volatilise slowly (Henry's Law constant of 1×10^{-7} to 1×10^{-6})	2
		• Volatile (Henry's Law constant of $>1 \times 10^{-6}$)	1

Criteria	Importance	Parameter	Weighting (1 low: 3 high)
Level of occurrence in wastewater (it is acknowledged that absence of evidence does not necessarily indicate that chemicals are not present)	This will provide an indication that these chemicals have been detected and that there may be greater likelihood of them being present in finished water. It is likely that this data will be limited; therefore, any occurrence will be a case for high priority.	• Any data on occurrence that indicates its presence.	3
Level of occurrence in raw water	This will provide an indication that these chemicals have been detected and that there may be greater likelihood of them being present in finished water. It is likely that these data will be limited; therefore, any occurrence will be a case for high priority.	• Any data on occurrence that indicates its presence.	3
Level of occurrence in drinking water	This will provide an indication that these chemicals have been detected and that there may be greater likelihood of them being present in finished water. It is likely that this data will be limited; therefore, any occurrence will be a case for high priority.	• Any data on occurrence that indicates its presence.	3
Usage statistics	This will provide a rough estimation of the amount of these chemicals that are used in PCPs and DCPs. Chemicals that have a higher likelihood of being used in large quantities are more likely to be present in finished water.	• Used or sold in the UK at amounts >1000 tonnes/year. • Used or sold in Europe at amounts >10 000 tonnes/year. • Used or sold globally or in the USA at amounts >100 000 tonnes/year	3 3 3
		• Used or sold in the UK at amounts <1000 tonnes/year. • Used or sold in Europe at amounts <10 000 tonnes/year. • Used or sold globally or in the USA at amounts <100 000 tonnes/year	1 1 1

Criteria	Importance	Parameter	Weighting (1 low: 3 high)
		• Manufactured in the UK at amounts >10 000 tonnes/year.	3
		• Manufactured in Europe at amounts >100 000 tonnes/year.	3
		• Manufactured globally or in the USA at amounts >1 000 000 tonnes/year	3
		• Manufactured in the UK at amounts <10 000 tonnes/year.	1
		• Manufactured in Europe at amounts <100 000 tonnes/year.	1
		• Manufactured globally or in the USA at amounts <1 000 000 tonnes/year	1
		• No usage data found.	2

Table 3.3 is a worked example of the scoring process and presents the data used for prioritisation and the subsequent score.

Table 3.3 Worked example of scoring for prioritisation

Parameter and scoring category	Data and score
Chemical name (common)	(1-hydroxyethylidene) diphosphonic acid (HEDP)
CAS number	2809-21-4
Main category	Phosphonate
CLP classifications	Acute Toxicity category 4, Irritant, Specific Target Organ Toxicity Single Exposure Category 3, Repeat Exposure Category 2
Toxicity score	*3*
Log Kow	-3.49
Log Kow score (WwTW)	3
Log Kow Score (WTW)	3
Water solubility	690000 mg/l

Parameter and scoring category	Data and score
Water solubility Score (WwTW)	*3*
Water solubility score (WTW)	*3*
Biodegradation standardised	Not biodegradable
Biodegradation score (WwTW)	*3*
Biodegradation score (WTW)	*3*
Hydrolysis	Stable to hydrolysis
Hydrolysis score	*3*
Photolysis	Stable to photolysis
Photolysis score	*3*
Henrys law constant (atm m^3/mol)	5×10^{-17}
Henry's law constant score	*3*
Occurrence in effluent, surface water or drinking water	No data
Occurrence water supply score	*2*
Occurrence surface water score	*2*
Occurrence waste water score	*2*
Usage	7067 tonnes/year used in Europe in DCPs
Usage score	*1*
Total prioritisation score	***37***

Note: Rows highlighted in blue indicate standardised data gathered from literature.

3.2.3 Initial prioritised list

After application of the prioritisation criteria listed in Table 3.2 all 692 chemicals were ranked according to their potential to reach drinking water supplies (See Appendix B). The ranked list was top and bottom heavy with the top part of the list containing the substances where data were available and the data indicated that it may have a higher potential to reach drinking water supplies. The bottom part of the table contains chemicals for which data were available but the data indicated a low potential for the chemical to reach drinking water supplies. There is a large list of chemicals in the middle of the table where no data were located for any of the relevant parameters. The median prioritisation ranking score for the entire list is 28.

The maximum score was 42 (benzotriazole) and the lowest was 21 (isopropyl palmitate). All chemicals that had a total combined score of 35 or above are listed in Table 3.4. Within the agreed scope of the project, approximately 30 chemicals were intended to be taken forward to the modelling stage of the project. Therefore, a cut off score of 35 was considered to provide a pragmatic threshold that included a suitable number of chemicals without having to perform any further prioritisation of chemicals within a scoring band.

Table 3.4 Chemicals with a combined score of 35 or above

	Chemical name (common)	CAS number	Main category	Ranking score
1	1,2,3-Benzotriazole	95-14-7	Benzotriazole	42
2	Boric acid	10043-35-3	Enzyme stabiliser	38
3	EDTA	6381-92-6	Chelating	38
4	1H-Benzotriazole, 4(or 5)-methyl-	29385-43-1	Benzotriazole	38
5	Pentasodium pentetate	140-01-2	Chelating	37
6	Sodium bicarbonate	144-55-8	Buffering agent	37
7	Sodium sulphate	7757-82-6	Bulking agent	37
8	Tetrasodium EDTA	64-02-8	Chelating	37
9	(1-hydroxyethylidene) diphosphonic acid	2809-21-4	Acids	37
10	Amino tris(methylene phosphonic acid)	6419-19-8	Acids	37
11	Diethylenetriamine penta(methylene phosphonic acid)	15827-60-8	Acids	37
12	2-(2-butoxyethoxy)ethanol (DEGBE)	112-34-5	Solvent	36
13	Secondary Alkane Sulphonate	68037-49-0	Anionic surfactant	36
14	Silicic acid, disodium salt (anhydrous)	6834-92-0	Buffering agent	36
15	Sodium chloride	7647-14-5	Bulking agent	36
16	Sulphamic acid	5329-14-6	Buffering agent	36
17	Methyldibromo glutaronitrile	35691-65-7	Preservative	36
18	Linear Alkylbenzene Sulphonate	68411-30-3	Anionic surfactant	35
19	Citric acid	77-92-9; 5949-29-1; 6132-04-3	Buffering agent	35
20	Cocamidopropyl betaine (cosmetic grade)	61789-40-0, 83138-08-3, 86438-79-1	Amphoteric surfactant	35
21	Cocamidopropyl betaine (technical grade)	4292-10-8	Amphoteric surfactant	35
22	Dimethyl phthalate	131-11-3	Phthalate	35
23	Diethylene glycol ethyl ether (DEGEE)	111-90-0	Humectant	35
24	Salicylic acid	69-72-7	Conditioning agent	35
25	Triethanolamine	102-71-6	Buffering agent	35
26	Fluorescent Brightener FWA-1	16090-02-1	Fluorescent whitening agent	35

	Chemical name (common)	CAS number	Main category	Ranking score
27	Propylene glycol	57-55-6	Humectant	35
28	para-Aminophenol	123-30-8, 51-78-5	Hair dye	35

It is noted that this list contains inorganic chemicals that will quickly dissociate in water to ions that are found ubiquitously in water and are therefore not considered to be of concern. Chemicals such as the sodium salts sodium chloride, sodium sulphate, sodium carbonate, sodium percarbonate, sodium bicarbonate, sodium fluoride and silicic acid, disodium salt have therefore been excluded.

The classes of chemicals that were identified in the literature (KIWA, 2004, Reif *et al.,* 2011, Janna *et al.,* 2011, Kanda *et al.,* 2003, Kasprzyk-Hordern *et al., 2009,* and Stuart *et al.,* 2012) as having a higher potential to reach drinking water supplies have been listed in the left-hand column of Table 3.5. Their corresponding ranked score derived from the prioritisation process from this work is listed in the right-hand column, and those highlighted in bold are within the top 28 chemicals in the prioritised list. At least one chemical from each group in this list has been included in the final prioritised list.

Table 3.5 Substances identified as being of current and potential concern

Chemical	Score achieved during prioritisation
Musks	29 (musk xylene, musk ketone, ambrettolide), 28 (tonalide) and 22 (galaxolide).
Parabens	34 (methyl paraben), 33 (propylparaben, ethylparaben), 31 (butylparaben).
Phthalates	**35,** (dimethyl phthalate, DMP) 34, (Bis(2-methoxyethyl) phthalate, DMEP), 32 (Diethyl phthalate, DEP), 30 (Di-isobutyl phthalate, DIBP 29 (Dibutyl phthalate, DBP), 28 (Bis(2-ethylhexyl) phthalate DEHP).
Triclosan	31
N,N-diethyl-meta-toluamide (DEET)	32
Benzophenones	34 to 27
Benzotriazole	**42**
Tolyltriazole	**38**
Siloxanes	29 (Siloxane D5), 28 (Siloxane D6), 27 (Siloxane D4 and Hexamethyldisiloxane)

3.2.4 Final prioritised chemical list

The initial list was examined to ensure that the final prioritised list contained as diverse a range of chemicals from different product types as possible, and that it also contains examples of the chemicals that could potentially reach drinking water, as identified in the literature and/or were identified as being of interest by the Drinking Water Inspectorate. This examination was undertaken to ensure that the list did not contain large numbers of similar chemicals used in similar products as this would significantly limit the amount of information this project could provide. Upon examination it was decided that no changes needed to be made as the chemicals identified were suitably diverse and non-repetitive. The final list is detailed in Table 3.6. The chemicals in this list were taken forward to the modelling stage.

Table 3.6 Final proposed prioritised list of chemicals

Chemical	CAS no.	Main category	Product types used in	Score
Cocamidopropyl betaine	61789-40-0, 83138-08-3, 86438-79-1	Amphoteric surfactant	Foam booster in shampoo, hand soap and cosmetics.	35
Linear Alkylbenzene Sulphonate	68411-30-3	Anionic surfactant	Detergents	35
Secondary Alkane Sulphonate	68037-49-0	Anionic surfactant	Detergents	36
Triclosan	3380-34-5	Antimicrobial	Soaps, deodorants, oral care, cleaning	31
Sulphamic acid	5329-14-6	Buffering agent	Cleaning, descaling, rust removing, denture cleaner	36
Triethanolamine	102-71-6	Buffering agent	pH balancer in PCPs such as lotions, cleansers and shampoos	35
EDTA derivatives (Inc. Tetrasodium EDTA)	64-02-8, 6381-92-6, 6381-92-6	Chelating	Cosmetics	37
Pentasodium pentetate	140-01-2	Chelating	Cosmetics	37
Salicylic acid	69-72-7	Conditioning agent	Dishwashing, laundry, household cleaners, cosmetic and body care	35
1,2,3-Benzotriazole	95-14-7	Corrosion inhibitor	Dishwashing	42
1H-Benzotriazole, 4(or 5)-methyl-	29385-43-1	Corrosion inhibitor	Dishwashing	38
Boric acid	10043-35-3	Enzyme stabiliser	Liquid fabric softeners, cosmetics and oral care products	38
Fluorescent Brightener FWA-1	16090-02-1	Fluorescent whitening agent	Laundry detergent to brighten clothing	35
para-Aminophenol	123-30-8, 51-78-5	Hair dye	Precursor to hair dye	35
Diethylene glycol ethyl ether (DEGEE)	111-90-0	Humectant (moisturising agent)	Solvent, cosmetics	35
Propylene glycol	57-55-6	Humectant (moisturising agent)	Cosmetics and PCPs (although also added to food so may remove from list)	35
DEET	134-62-3	Insect repellents	Applied to skin and clothes	32

Chemical	CAS no.	Main category	Product types used in	Score
Musk ketone	81-14-1	Musks	Fragrance	29
Musk xylene	81-15-2	Musks	Fragrance	29
Methyl paraben	99-76-3	Paraben	Cosmetics and PCPs	34
Sodium Isopropylparaben	35285-69-9	Paraben	Cosmetics and PCPs	34
Sodium Methylparaben	5026-62-0	Paraben	Cosmetics and PCPs	34
(1-hydroxyethylidene) diphosphonic acid (HEDP)	2809-21-4	Phosphonate	Dish, laundry and household cleaning	37
Amino tris(methylene phosphonic acid) (ATMP)	6419-19-8	Phosphonate	Dish, laundry and household cleaning	37
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	15827-60-8	Phosphonate	Dish, laundry and household cleaning	37
Bis(2-methoxyethyl) phthalate	117-82-8	Phthalate/ fragrance	Cosmetics	34
Dimethyl phthalate	131-11-3	Phthalate/ fragrance	Cosmetics	35
Methyldibromo glutaronitrile	35691-65-7	Preservative	Detergents and polishing products	36
Siloxane (D4, D5, D6)	-	Skin Protectant	Cosmetics	27-29
2-(2-butoxyethoxy)ethanol (DEGBE)	112-34-5	Solvent	Household cleaners	36
Benzophenones	-	UV Sunscreen	Cosmetics	27-34

4. Stage 2: Potential to reach water supply

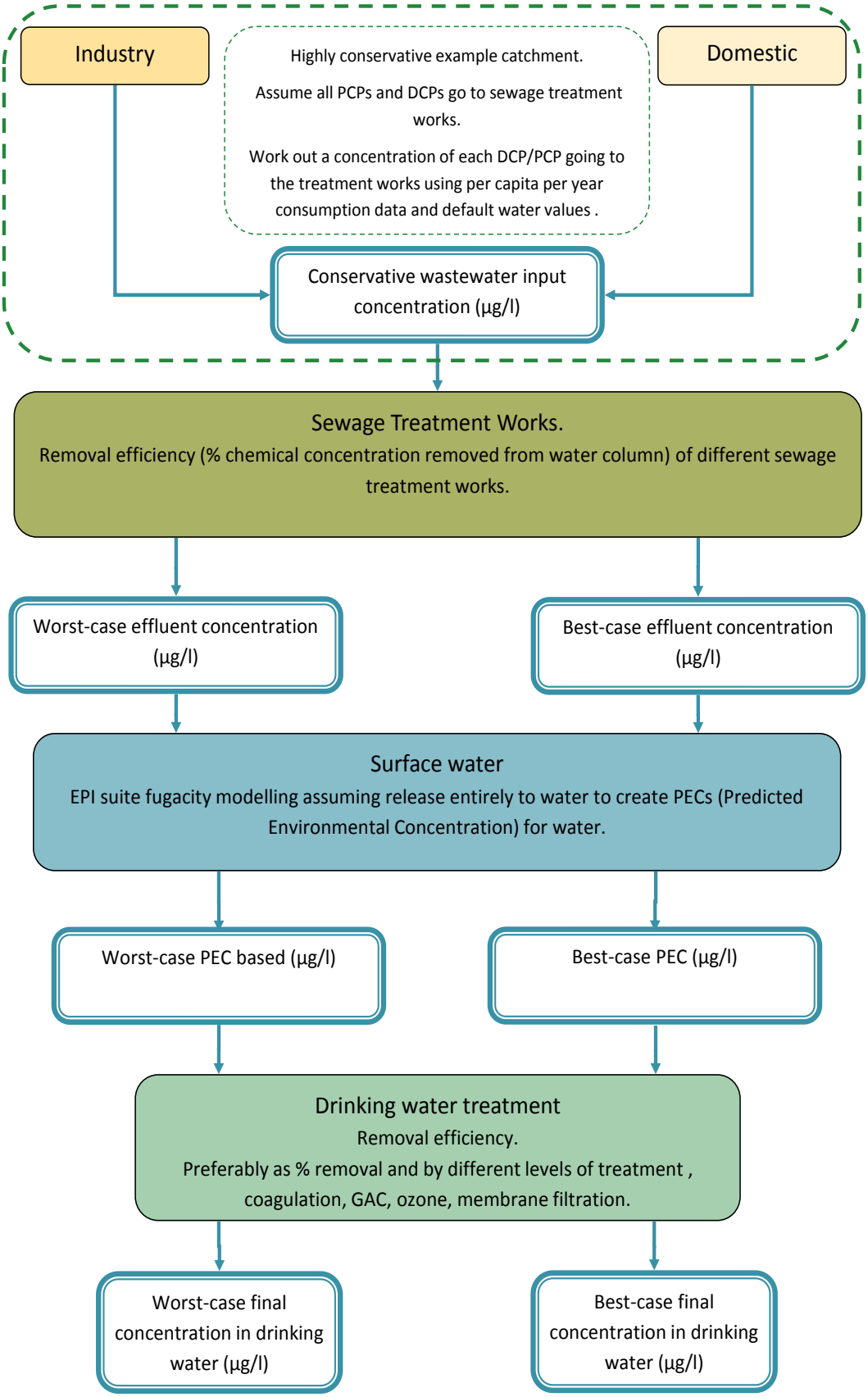
4.1 Model description

To predict the potential concentrations of these prioritised chemicals in drinking water a simple model was created. It was assumed that all of the PCPs and DCPs used within the UK will enter the sewerage system. This usage data was derived from the data provided by Euromonitor as this was the most up to date and comprehensive chemical usage dataset. These values include all the PCP and DCP ingredient tonnages used during manufacture, consumer use and commercial use. This is considered a worst case assessment. The amounts of PCPs and DCPs that reach landfill are very difficult to estimate and once in landfill may, or may not, migrate to ground water or surface water, again this value is difficult to predict. It is also difficult to estimate the quantities of PCPs and DCPs released to the atmosphere, but based on their known chemical structures it is reasonable to assume that this value would be very small. The model predicts the removal of these ingredients from the water column through wastewater treatment, environmental partitioning and potable water treatment resulting in a concentration in the finished drinking water.

The output from the model, a potential concentration in drinking water, is used to predict how much of each chemical people will be exposed to during drinking water and bathing. This exposure is then compared to the exposure people will be subjected to during typical use of the PCP or DCP product. Chemicals that have an estimated human exposure via drinking water and bathing greater than the estimated exposure through typical use of the PCP or DCP products will be identified as chemicals that potentially require further investigation.

Figure 4.1 is a flow diagram of the model developed to predict the potential concentration of the prioritised chemicals in drinking water.

Figure 4.1 Flow diagram of model designed to estimate potential concentrations in drinking water



4.1.1 UK usage data

The amount of exposure during the intended use of these products provides some indication of the relative level of risk from unintended sources, and there is greater likelihood of occurrence in water if the initial usage is higher. Usage trends are important for forecasting what may occur in the future.

Euromonitor are a market research company who collate market share data for various purposes including ingredients used in PCPs and DCPs. Euromonitor have provided annual consumption tonnages for ingredients used in these market sectors within the UK from 2007 to 2012. It has been assumed, for the purposes of this assessment, that the entire production tonnage of each ingredient (used within these sectors) is used and sold within the UK. It is likely that products and ingredients are imported and exported outside of the UK. This is also conservative as some of these products may be bought within the UK yet only used abroad, for example products such as sunscreens and insect repellents may be used whilst people are on holiday. However, it is also possible that there are products imported into the UK from elsewhere but it is not possible to estimate this addition to the consumption in the UK.

Specific information was available for some ingredients, such as EDTA and linear alkylbenzene sulphonates, but for other ingredients the use data relates to category types of ingredients such as “parabens” or “ethoxylated fatty acids”. If a specific ingredient has not been named in the Euromonitor data then the category type usage data has been used. In each instance, for each chemical on our prioritisation list, it has been assumed that the full production tonnage in a group is made up equally by number of ingredients in the category (e.g. there are three parabens on the prioritised list within the group “Parabens” each paraben in our prioritisation list has been assessed using one third of the full tonnage for the group). This is a pragmatic estimation as it is not possible to tell from this data the exact tonnages for each individual chemical.

Table 4.1 Ingredient categories assigned to each chemical in the prioritisation list

Chemical	Main Category	Euromonitor Category
Secondary Alkane Sulphonate	Anionic surfactant	Alkane sulphonates
Triethanolamine	Buffering agent	Alkanolamines
Cocamidopropyl betaine	Amphoteric surfactant	Alkyl amido alkyl betaines
Benzophenones	UV Sunscreen	Benzophenone
Pentasodium pentetate	Chelating	Carboxylates
EDTA derivatives (Inc. Tetrasodium EDTA)	Chelating	Ethylenediamine Tetraacetic Acid and Salts
Fluorescent Brightener FWA-1	Fluorescent whitening agent	Fluorescers
Musk ketone	Musks	Fragrances
Musk xylene	Musks	Fragrances
Bis(2-methoxyethyl) phthalate	Phthalate/ fragrance	Fragrances

Chemical	Main Category	Euromonitor Category
Dimethyl phthalate	Phthalate/ fragrance	Fragrances
N,N-Diethyl-m-toluamide (DEET)	Insect repellents	Insect Repellents
Linear Alkylbenzene Sulphonate	Anionic surfactant	Linear Alkylbenzene Sulphonate
Sulphamic acid	Buffering agent	Other Acidulants
Boric acid	Enzyme stabiliser	Other Acidulants
1,2,3-Benzotriazole	Corrosion inhibitor	Other Miscellaneous Ingredients
1H-Benzotriazole, 4(or 5)-methyl-	Corrosion inhibitor	Other Miscellaneous Ingredients
Methyldibromo glutaronitrile	Preservative	Other Preservatives/Antioxidants
Methyl paraben	Paraben	Parabens
Sodium isopropylparaben	Paraben	Parabens
Sodium methylparaben	Paraben	Parabens
para-Aminophenol	Hair dye	Permanent/oxidative hair dyes
(1-hydroxyethylidene) diphosphonic acid (HEDP)	Phosphonate	Phosphonates
Amino tris(methylene phosphonic acid) (ATMP)	Phosphonate	Phosphonates
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	Phosphonate	Phosphonates
Diethylene glycol ethyl ether (DEGEE)	Humectant	Polyalkylene Glycols
2-(2-butoxyethoxy)ethanol (DEGBE)	Solvent	Polyalkylene Glycols
Propylene glycol	Humectant (moisturising agent)	Propylene glycol
Salicylic acid	Conditioning agent	Salicylic acid and its salts
Siloxane (D4-octamethylcyclotetrasiloxane)	Skin Protectant	Silicones (Antifoams)
Siloxane (D5-decamethyl-cyclopentasiloxane)	Skin Protectant	Silicones (Antifoams)

The ingredients with the highest consumption in the UK are linear alkylbenzene sulphonates (LAS), which are anionic surfactants that are commonly used in most PCPs and DCPs (~50 000 tonnes/year since 2007). Other surfactants such as cocamidopropyl betaine and secondary alkane sulphonates (SAS) are also high on the consumption list. Surfactants are used in a wide range of products such as detergents, laundry products, dishwashing products, soaps and shampoos. Fragrance ingredients and acidic chemicals are also used in large quantities in the UK, however the number of different fragrances and acidic chemicals used is vast and these have been grouped under single consumption figures. Not unexpectedly,

ingredients used in dish and laundry cleaning generally have high consumption tonnages (500 to 2500 tonnes/year). Humectants (substances that help a product retain water) and skin protectants are used in quite large quantities (2500 to 4500 tonnes/year) as they are widely used in PCPs such as soaps, moisturisers and shampoos and some DCPs, such as hand dishwashing liquids. Ingredients with lower consumption include benzophenones, insect repellents and preservatives (5 to 12 tonnes/year) (See Table 4.2, Table 4.3 and Table 4.4).

Table 4.2 UK Consumption of ingredients used in both PCPs and DCPs

Chemical	Type of product used in	UK consumption (tonnes/year)					
		2007	2008	2009	2010	2011	2012
Linear Alkylbenzene Sulphonate	Anionic surfactant, Detergents	48782	49778	53410	52734	51009	50530
Bis(2-methoxyethyl) phthalate	Phthalate, Fragrance	625	636	653	669	679	690
Dimethyl phthalate	Phthalate, Fragrance	625	636	653	669	679	690
Musk ketone	Musks, Fragrance	625	636	653	669	679	690
Musk xylene	Musks, Fragrance	625	636	653	669	679	690
Boric acid	Enzyme stabiliser Liquid fabric softeners, cosmetics and oral care products	586	519	745	783	827	841
Sulphamic acid	Buffering agent. Cleaning, descaling, rust removing, denture cleaner	586	519	745	783	827	841
Secondary Alkane Sulphonate	Anionic surfactant, Detergents	265	263	245	218	212	206
Salicylic acid	Conditioning agent, Dishwashing, laundry, household cleaners, cosmetic and body care	12	13	11	18	19	21

Table 4.3 UK Consumption of ingredients used in PCPs

Chemical	Type of product used in	UK consumption (tonnes/year)					
		2007	2008	2009	2010	2011	2012
Cocamidopropyl betaine	Amphoteric surfactant. Foam booster in shampoo, hand soap and cosmetics.	4604	4813	6025	6484	6644	6863
Diethylene glycol ethyl ether (DEGEE)	Humectant (moisturising agent), solvent. Cosmetics.	2310	2360	2356	2242	2127	2040
Propylene glycol	Humectant (moisturising agent) Cosmetics and PCPs.	2589	2186	3020	3112	3131	3140

Chemical	Type of product used in	UK consumption (tonnes/year)					
		2007	2008	2009	2010	2011	2012
Triethanolamine	Buffering agent pH balancer in PCPs such as lotions, cleansers and shampoos.	409	419	364	369	373	370
EDTA derivatives (Inc. Tetrasodium EDTA)	Chelating. Cosmetics.	259	261	254	260	262	269
Methyl paraben	Paraben. Cosmetics and PCPs	54	56	56	56	55	58
Sodium isopropylparaben	Paraben. Cosmetics and PCPs	54	56	56	56	55	58
Sodium methylparaben	Paraben. Cosmetics and PCPs	54	56	56	56	55	58
para-Aminophenol	Hair dye. Precursor to hair dye	97	97	105	111	118	126
Siloxane D4	Skin protectant, cosmetics	52	53	54	53	54	38
Siloxane D5	Skin protectant, cosmetics	52	53	54	53	54	38
Siloxane D6	Skin protectant, cosmetics	52	53	54	53	54	38
Triclosan	Antimicrobial soaps, deodorants, oral care, cleaning	48	47	58	59	60	62
Benzophenones	UV sunscreen cosmetics	5	6	9	16	17	18
Pentasodium pentetate	Chelating. Cosmetics	8	8	8	7	8	8
N,N-Diethyl-m-toluamide (DEET)	Insect repellents. Applied to skin and clothes	7	7	7	7	7	7

Table 4.4 UK Consumption of ingredients used in DCPs

Chemical	Type of product used in	UK consumption (tonnes/year)					
		2007	2008	2009	2010	2011	2012
2-(2-butoxyethoxy)ethanol (DEGBE)	Solvent. Household cleaners	2310	2360	2356	2242	2127	2040
(1-hydroxyethylidene) diphosphonic acid (HEDP)	Phosphonate. Dish, laundry and household cleaning.	2310	2360	2356	2242	2127	2040
Amino tris(methylene phosphonic acid) (ATMP)	Phosphonate. Dish, laundry and household cleaning.	2310	2360	2356	2242	2127	2040
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	Phosphonate. Dish, laundry and household cleaning.	2310	2360	2356	2242	2127	2040
1,2,3-Benzotriazole	Corrosion inhibitor. Dishwashing	832	762	698	619	495	390
1H-Benzotriazole, 4(or 5)-methyl-	Corrosion inhibitor. Dishwashing	832	762	698	619	495	390
Fluorescent Brightener FWA-1	Fluorescent whitening agent. Laundry detergent.	472	451	436	399	346	307
Methyldibromo glutaronitrile	Preservative. Detergents and polishing products.	7	10	15	17	18	19

4.1.2 Initial input concentration of chemicals

To model the potential concentrations of each chemical in drinking water, the most recent (2012) usage data was used (See Table 4.6). As the values supplied by Euromonitor are total consumption values for the whole of the UK (in the PCP and DCP market) these values were converted to “per capita” values, assuming that each product is used equally across the entire population of the UK. It is known that different populations of different geographical areas, ages and genders will use some products more than others. No data were located that provided such a detailed breakdown for each ingredient consumption tonnage for 2012. Therefore, the total amount was divided by the latest population figures (63 182 000 people) produced by the Office for National Statistics[1] for 2007 and converted to an ‘amount of ingredient used per person per year’ in kg. This per capita amount was then converted to a potential concentration in µg/l. It was assumed that each person uses the products equally across all 365 days in a year and that each person produces a standard 200 litres of wastewater per day (See Table 4.6). Historically, 200 litres per day has been used as a best estimate of water usage per person per day. However, it is noted that with increased pressure for water efficiency this figure may have decreased and is expected to decrease further in the future. This will potentially increase the input concentrations of these chemicals to the wastewater treatment works (WwTW).

4.1.3 Wastewater Treatment

The removal of ingredients from the water column during wastewater treatment was modelled using data from various sources (See Appendix B). The data on removal during wastewater treatment was highly varied for each chemical on the prioritised list. There were no common themes as to the type of processes assessed. The data were collated into a spreadsheet that details the minimum and maximum removal that has been reported in the literature and the fate of the chemical within the treatment works (i.e. amount of the input concentration sorbs to sludge, the amount that is biodegraded and amount that is anticipated to remain in the water column). These removal rates were then applied to the input concentration to estimate the concentration of PCPs and DCPs in effluent that would be released to surface water. In this case, a maximum (worst case) and minimum (best case) concentration that could be achieved through wastewater treatment can be estimated.

4.1.4 Environmental Fugacity Modelling

To estimate the distribution in the environment, a Mackay Level III Fugacity Model (US EPA/SRC EpiSuite programme version 4.1) was used to estimate the distribution between the water phase, the air, sediment and soil (US EPA/SRC, 2011). These are given in percentages to each phase. These percentages were applied to the best [lowest] and worst [highest] concentrations coming from effluent at the wastewater treatment works to predict the lowest and highest concentrations that could potentially reach drinking water treatment.

[1] Office for national statistics website.

The EPI Suite model was run using the measured physico-chemical property values collected during the literature search stage of the project rather than the estimates that would otherwise be generated by the programme. If data were not located for a specific physico-chemical parameter value, then the EPI Suite estimates were used. For grouped chemicals such as benzophenones and EDTA and its derivatives, a fugacity model was created for each chemical within that group then the average distribution in air, water, soil and sediment was taken for the group.

Table 4.5 Physico-chemical parameters used in the fugacity modelling

Chemical	Log Kow	Boiling Point (°C)	Melting Point (°C)	Vapor Pressure (mm Hg)	Water Solubility (mg/L)	Henry LC (atm-m3/mole)
(1-hydroxyethylidene) diphosphonic acid (HEDP)	-3.49	*456.79*	195.00	$1.24x10^{-10}$	$6.90x10^{5}$	$5.00x10^{-17}$
1,2,3-Benzotriazole	1.44	350.00	100.00	$2.40x10^{-5}$	$1.98x10^{4}$	$1.47x10^{-7}$
1H-Benzotriazole, 4(or 5)-methyl-	1.71	160.00	76.00	$2.08x10^{-4}$	$3.07x10^{3}$	$1.62x10^{-7}$
2-(2-butoxyethoxy)ethanol (DEGBE)	0.56	231.00	-68.00	$2.19x10^{-2}$	$1.00x10^{6}$	$7.20x10^{-9}$
Amino tris(methylene phosphonic acid) (ATMP)	-3.53	480.00	90.30	$6.86x10^{-12}$	$1.00x10^{6}$	$8.00x10^{-18}$
Benzophenone	3.18	305.40	48.50	$1.93x10^{-3}$	$1.37x10^{2}$	$1.94x10^{-6}$
Benzophenone-1	2.96	*374.59*	144.00	$1.41x10^{-5}$	$2.36x10^{2}$	$2.00x10^{-10}$
Benzophenone-2	2.78	*444.26*	200.00	$4.94x10^{-10}$	$3.99x10^{2}$	$2.01x10^{-10}$
Benzophenone-3	3.79	*155.00*	65.50	$1.42x10^{-6}$	$6.86x10^{1}$	$2.01x10^{-10}$
Benzophenone-4	0.37	*497.59*	145.00	$1.34x10^{-11}$	$2.50x10^{5}$	$7.03x10^{-15}$
Benzophenone-5	*-1.42*	*698.28*	*305.22*	*$6.42x10^{-18}$*	*$3.98x10^{2}$*	*$7.06x10^{-15}$*
Benzophenone-6	3.90	*421.90*	139.50	$7.37x10^{-9}$	$2.70x10^{1}$	$1.97x10^{-9}$
Benzophenone-7	*4.09*	*358.45*	93.00	*$4.69x10^{-6}$*	*$1.01x10^{3}$*	*$1.89x10^{-7}$*
Benzophenone-8	3.82	*398.24*	68.00	$1.94x10^{-7}$	$1.62x10^{2}$	$1.97x10^{-9}$
Benzophenone-9	*-2.78*	*852.10*	*349.84*	*$1.57x10^{-24}$*	*$1.88x10^{2}$*	*$2.57x10^{-23}$*
Benzophenone-10	4.07	*375.01*	*140.83*	$5.36x10^{-7}$	$3.30x10^{1}$	$1.66x10^{-8}$
Benzophenone-12	6.96	*273.50*	48.50	$6.92x10^{-8}$	$1.75x10^{-1}$	$2.18x10^{-10}$
Bis(2-methoxyethyl) phthalate	1.11	*340.00*	-45.00	$2.28x10^{-4}$	$8.50x10^{3}$	$2.81x10^{-13}$
Boric acid	0.18	*616.55*	170.90	$5.24x10^{-18}$	$5.00x10^{4}$	$2.60x10^{-12}$
Cocamidopropyl betaine	-1.28	*600.00*	260.00	$1.50x10^{-13}$	$8.77x10^{3}$	$3.95x10^{-20}$
DEET	2.18	*290.00*	-45.00	$2.00x10^{-3}$	$9.12x10^{2}$	$2.08x10^{-8}$
Diethylene glycol ethyl ether (DEGEE)	-0.54	*196.00*	-76.00	$1.26x10^{-1}$	$1.00x10^{6}$	$5.72x10^{-11}$
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	-3.40	*480.00*	200.00	$1.25x10^{-12}$	$5.00x10^{5}$	$7.30x10^{-18}$
Dimethyl phthalate	1.60	283.70	5.50	$3.08x10^{-3}$	$4.00x10^{3}$	$1.97x10^{-7}$
EDTA	-3.86	*557.81*	245.00	$1.50x10^{-12}$	$1.00x10^{3}$	$5.77x10^{-16}$
tetrasodium EDTA	-13.17	*572.70*	300.00	$1.49x10^{-12}$	$5.00x10^{5}$	$1.18x10^{-23}$
trisodium EDTA	-13.15	*692.95*	*335.12*	$7.81x10^{-17}$	$1.00x10^{6}$	$1.18x10^{-23}$
Fluorescent Brightener FWA-1	-1.58	*1188.28*	300.00	$5.25x10^{-18}$	$1.80x10^{3}$	$1.18x10^{-23}$

Chemical	Log Kow	Boiling Point (°C)	Melting Point (°C)	Vapor Pressure (mm Hg)	Water Solubility (mg/L)	Henry LC (atm-m3/mole)
Linear Alkylbenzene Sulphonate	3.32	*637.00*	277.00	$1.30x10^{1}$	$2.50x10^{5}$	$6.35x10^{-3}$
Methyl paraben	1.96	*275.00*	131.00	$2.37x10^{-4}$	$2.50x10^{3}$	$2.16x10^{-8}$
Methyldibromo glutaronitrile	1.63	*327.79*	52.00	$5.03x10^{-5}$	$1.30x10^{3}$	$3.90x10^{-10}$
Musk ketone	4.30	*401.75*	135.50	$4.00x10^{-5}$	$4.60x10^{-1}$	$1.29x10^{-12}$
Musk xylene	4.45	*411.56*	110.00	$6.35x10^{-7}$	$4.72x10^{-1}$	$8.31x10^{-13}$
para-Aminophenol	0.04	284.00	187.50	$4.00x10^{-5}$	$1.60x10^{4}$	$3.60x10^{-10}$
Pentasodium pentetate	-16.25	105.60	*286.24*	$2.85x10^{-15}$	$1.00x10^{6}$	$1.16x10^{-30}$
Propylene glycol	-0.92	187.60	-60.00	$1.29x10^{-1}$	$1.00x10^{6}$	$1.29x10^{-8}$
Salicylic acid	2.26	211.00	159.00	$8.20x10^{-5}$	$2.24x10^{3}$	$7.34x10^{-9}$
Secondary Alkane Sulphonate	2.76	*599.68*	200.00	$3.98x10^{-13}$	$3.00x10^{5}$	*$5.03x10^{-7}$*
Siloxane D4 (octamethylcyclotetrasiloxane)	6.74	175.80	17.50	1.05	$5.60x10^{-2}$	$1.20x10^{1}$
Siloxane D5 (decamethylcyclopentasiloxane)	8.03	210.00	-38.00	$2.00x10^{-1}$	$1.70x10^{-2}$	$3.30x10^{1}$
Siloxane D6 (decamethylcyclopentasiloxane)	9.06	245.00	-3.00	$1.64x10^{-2}$	$5.10x10^{-3}$	$4.89x10^{1}$
Sodium Isopropylparaben	-0.36	*511.76*	*218.09*	$1.20x10^{-10}$	$8.59x10^{4}$	$1.14x10^{-8}$
Sodium Methylparaben	1.96	*275.00*	131.00	$8.55x10^{-4}$	$2.50x10^{3}$	$3.61x10^{-9}$
Sulphamic acid	0.10	*260.00*	205.00	$3.21x10^{-16}$	$1.47x10^{5}$	$4.26x10^{-9}$
Triclosan	4.76	*290.00*	54.00	$6.45x10^{-7}$	$1.00x10^{1}$	*$2.46x10^{-8}$*
Triethanolamine	-1.00	*335.40*	20.50	$3.59x10^{-6}$	$1.00x10^{6}$	$7.05x10^{-13}$

Italicised data points were estimated by the EPI Suite model.

It should be noted that the following assumptions have been made during this stage of the modelling:

- the only source of these chemicals going to environment is the wastewater treatment works effluent emission to surface water (i.e. 100% of the chemical is released to surface water, ground water is not considered in this model);
- there has been no consideration of the effects of dilution in the environment, it is likely that there will be significant dilution of these chemicals in UK rivers prior to abstraction for drinking water treatment;
- only the advection (i.e. distribution between air, water, soil and sediment) aspect of the model has been used for this project to estimate losses from water, the biodegradation aspect of the model has not been included within these predictions; and
- abiotic degradation processes such as hydrolysis and photolysis have not been taken into account.

The prioritisation process will tend to favour those chemicals that are less likely to undergo environmental degradation processes such as biodegradation, hydrolysis and photolysis, and so omitting these factors from the modelling is a reasonable assumption.

Omitting the consideration of dilution in the environment provides what may be considered to be an extreme "worst-case" assessment of potential concentrations in the environment. Generic exposure assessment models, such as EUSES (EUSES 2.1.2 version, 2012), often apply a minimum dilution factor of 10, but this may not be appropriate for the whole of the UK.

Deriving a suitable dilution factor for the whole of the UK is difficult, as reported by Keller *et al.* (2014). The variability in the concentrations of these compounds in the environment is driven by seasonal variability in river flows, and in demographic variability such as population density. This variability in the UK is particularly marked due to the large variation in seasonal river flows and the large differences in population densities, such as between the South East and the Highlands of Scotland. Keller *et al.,* (2014) reported that within the UK calculated dilution factors between locations can differ between 10 and 1000 (with 95th percentile ranges between 1 and 10 000) and that the data is skewed towards low dilution factors in areas with high population densities. The reported average dilution factor for the UK was between 10 and 40 but this was considered misleading due to the large variation between locations. Therefore, as an initial screen it is considered appropriate to assume no dilution in the environment. Any subsequent comparisons via drinking water with other routes of exposure will therefore overestimate the importance of exposure via drinking water. Therefore, if exposure via drinking water is not considered to be a significant source of exposure based on these conservative assumptions there is likely to be an even greater "margin of safety" than the estimates would suggest. However, if exposure via drinking water is indicated to be higher than via other routes of exposure, this does not indicate a concern *per se*, but would indicate that further refinement for these chemicals, such as a 10 fold dilution in the environment, to reflect more realistic environmental considerations may be appropriate.

4.1.5 Drinking Water Treatment

The potential removal efficiency of various treatment processes for the chemicals on the prioritised chemicals list was derived using the chemical structure and physico-chemical properties of each chemical. Removal efficiencies for treatment using coagulation, Granular Activated Carbon (GAC), Ozone, and membrane filtration, were derived and combined to create five different scenarios for different levels of treatment.

1. Coagulation
2. GAC
3. Coagulation and GAC
4. Coagulation, GAC and ozone
5. Coagulation, GAC, ozone and membrane filtration

The assumptions made for each chemical and its fate during treatment are laid out in Appendix D.

The best [lowest] and worst [highest] concentrations coming from the surface water are then used with these different scenarios to estimate the potential range of concentrations in potable water supplies.

In most cases a 0% removal was applied to the maximum surface water concentration to generate the maximum drinking water concentration.

4.2 Comparison of reported occurrence data with modelled occurrence

4.2.1 Modelled concentration values

The modelled concentrations in WwTW effluent, surface water and finished drinking water are presented in Table 4.6. The maximum concentration estimates represent a worst-case concentration prediction for the model, as they are based on the lowest levels of removal of PCPs and DCPs during sewage and drinking water treatment. The minimum concentration estimates represent a best-case concentration prediction for the model, as they are based on estimates of the highest levels of removal at both the wastewater treatment works and at the drinking water treatment works. These values have been compared to actual measured data in Section 4.2.2, Section 0 and Section 4.2.4.

It is noted that the predicted concentrations of boric acid, sulphamic acid and linear alkylbenzene sulphonate in drinking water are the highest of all the compounds modelled. It appears that boric and sulphamic acids have little removal from the water column during waste water and drinking water treatment. The initial concentrations of these acids are likely to be overestimated because the category group that was most appropriate was “other acidulants” which contains the usage volumes of a number of other acids. Linear alkylbenzene sulphonate had the highest usage volume of all the ingredients listed in the Euromonitor dataset. However linear alkylbenzene sulphonate is biodegradable and this is reflected in the high removal in STW that is not accounted for in the environmental compartment of the model. Even if an allowance were made for biodegradability, it is likely a high concentration will potentially reach drinking water.

Table 4.6 Concentrations predicted at various stages of the model

Chemical	Influent	Effluent		Surface water		Drinking water	
	Concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)
(1-hydroxyethylidene) diphosphonic acid (HEDP)	103	20.6	10.3	20.5	10.3	20.5	10.3
1,2,3-Benzotriazole	84.5	60.4	37.9	60.0	37.7	60.0	3.77
1H-Benzotriazole, 4(or 5)-methyl-	84.5	20.4	11.5	20.3	11.4	20.3	1.14
2-(2-butoxyethoxy)ethanol (DEGBE)	442.3	57.5	44.2	57.4	44.1	57.4	44.1
Amino tris(methylene phosphonic acid) (ATMP)	103	20.6	7.20	20.4	7.15	20.4	7.15
Benzophenones	3.90	1.48	0.04	1.34	0.04	1.34	0.01
Bis(2-methoxyethyl) phthalate	150	2.99	2.99	2.98	2.98	2.98	1.49
Boric acid	182	182	137	182	136	182	136
Cocamidopropyl betaine	1488	149	0.00	145	0.0	145	0.0
Diethylene glycol ethyl ether (DEGEE)	442	173	8.85	172	8.83	172	8.83
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	103	15.4	3.08	3.47	0.69	3.47	0.69
Dimethyl phthalate	150	10.5	5.98	10.4	5.96	8.34	0.60
EDTA derivatives (Inc. Tetrasodium EDTA)	58.3	58.3	58.3	57.8	57.8	57.8	5.78
Fluorescent Brightener FWA-1	66.6	10.0	6.66	0.11	0.08	0.11	0.03

Chemical	Influent	Effluent		Surface water		Drinking water	
	Concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)	Maximum concentration (µg/l)	Minimum concentration (µg/l)
Linear Alkylbenzene Sulphonate	10956	1205	110	1030	93.7	1030	46.8
Methyl paraben	12.7	2.79	0.13	2.77	0.13	2.77	0.05
Methyldibromo glutaronitrile	4.18	4.14	4.14	4.13	4.13	4.13	3.71
Musk ketone	150	29.9	9.01	25.4	7.66	20.3	3.06
Musk xylene	150	57.3	6.03	11.5	1.21	9.17	0.48
N,N-Diethyl-m-toluamide (DEET)	1.58	1.58	0.14	1.57	0.14	1.57	0.08
para-Aminophenol	27.2	3.54	2.18	3.52	2.17	3.52	1.08
Pentasodium pentetate	1.67	1.67	1.67	1.55	1.55	1.55	1.09
Propylene glycol	681	54.5	3.40	54.4	3.40	54.4	3.40
Salicylic acid	4.44	0.13	0.07	0.13	0.07	0.13	0.03
Secondary Alkane Sulphonate	44.7	1.34	0.04	1.29	0.04	1.29	0.03
Siloxane (D4-octamethylcyclotetrasiloxane)	8.14	0.81	0.16	0.45	0.09	0.45	0.04
Siloxane (D5-decamethyl-cyclopentasiloxane)	8.14	0.73	0.16	0.36	0.08	0.36	0.04
Siloxane (D6-dodeca-methylcyclohexasiloxane)	8.14	0.81	0.24	0.38	0.11	0.38	0.06
Sodium isopropylparaben	12.7	2.79	0.38	2.75	0.38	2.75	0.23
Sodium methylparaben	12.7	2.79	0.13	2.77	0.13	2.77	0.08
Sulphamic acid	182	182	182	182	182	182	182
Triclosan	13.4	2.81	0.94	1.01	0.34	1.01	0.10
Triethanolamine	80.3	9.63	4.82	9.61	4.81	9.61	4.81

4.2.2 Modelled Effluent Concentrations

There were limited data available in the literature on the concentrations of these PCPs and DCPs in effluent. The available data have been summarised in Table 4.7 and compared to the modelled values. Where multiple values have been found the maximum measured occurrence value has been used.

As shown in Table 4.7, modelled estimates for effluent concentration of 2-(2-butoxyethoxy)ethanol (DEGBE), benzotriazoles, linear alkylbenzene sulphonates (LAS), musk ketone and musk xylene are highly conservative, with estimated concentrations between 10 and 20 times higher than the measured concentrations.

However, estimated concentrations of EDTA, salicylic acid, secondary alkane sulphonate (SAS) and siloxanes are all below the literature maximum values. This may be due additional inputs of these chemicals to sewage that are not considered within the scope of this model, for example, salicylic acid is also a pharmaceutical. It is also possible that the maximum measured values have arisen in response to a specific contamination event in which case elevated concentrations would be expected.

The estimated concentrations of benzophenones and the minimum effluent concentration for musk xylene are approximately the same as the reported concentrations for these chemicals in the literature.

Table 4.7 Modelled concentrations in effluent versus measured effluent concentrations from literature

Chemical	Maximum predicted concentration in effluent (µg/l)	Minimum predicted concentration in effluent (µg/l)	Measured concentration for effluent (µg/l)	References
1,2,3-Benzotriazole	60.4	37.9	3.61	Janna *et al*, (2011).
1H-Benzotriazole, 4(or 5)-methyl-	20.4	11.5	5.70	Janna *et al*, (2011).
2-(2-butoxyethoxy)ethanol (DEGBE)	57.5	44.2	9.00	EC, (1999).
Benzophenones	1.48	0.04	1.00	EC, (2013).
EDTA derivatives, Inc. Tetrasodium EDTA)	58.3	58.3	5000	EC, (2004).
Linear Alkylbenzene Sulphonate	1205	110	273	HERA, (2009).
Musk ketone	29.9	9.01	0.71	OSPAR Commission, (2004).
Musk xylene	57.3	6.03	5.00	EC, (2005).

Chemical	Maximum predicted concentration in effluent (µg/l)	Minimum predicted concentration in effluent (µg/l)	Measured concentration for effluent (µg/l)	References
Salicylic acid	0.13	0.07	19.0	IUCLID, (2000e).
Secondary Alkane Sulphonate	1.34	0.04	8.00	HERA, (2005a).
Siloxane (D5-decamethyl-cyclopentasiloxane)	0.73	0.16	26.7	Health Canada, (2008a).
Siloxane (D6-dodeca-methylcyclohexasiloxane)	0.81	0.24	2.71	Swedish Environmental Research Institute, (2005).
No data available for remaining compounds				

4.2.3 Environmental Concentrations

The data available in the literature on the concentrations of these chemicals in environmental waters (surface water and ground water) were limited. The available data have been summarised in Table 4.8 and compared to the modelled values. Where multiple values have been found the maximum measured occurrence value has been used.

Modelled concentrations for benzotriazoles, boric acid, linear alkylbenzene sulphonate, musks, DEET and siloxane D6 were higher than measured concentrations in natural waters from the literature.

Dimethyl phthalate, fluorescent brightener FWA-1, propylene glycol and triclosan were all reported at greater concentrations in the literature than from the modelling. This may be due to sources of input into environmental water other than from their use in PCPs and DCPs, e.g. propylene glycol is used in many industries and for a range of applications. A further factor may be that the measured concentrations were analysed in response to a contamination event.

The estimations for benzophenones, EDTA, salicylic acid, secondary alkane sulphonate and siloxane D4 and D5 were generally similar to the measured values in the literature.

Table 4.8 Modelled concentrations in raw water versus measured surface water concentrations from literature

Chemical	Maximum predicted concentration in surface water (µg/l)	Minimum predicted concentration in surface water (µg/l)	Measured concentrations for surface water (µg/l)	References
1,2,3-Benzotriazole	60.0	37.7	3.69	Voutsa *et al*, (2006).
1H-Benzotriazole, 4(or 5)-methyl-	20.3	11.4	1.20	Janna *et al*, (2011).
Benzophenones	1.34	0.04	2.13	IUCLID, (2000a).
Boric acid	182	136	13.0	HERA, (2005b).
Dimethyl phthalate	10.4	5.96	11.0	IUCLID, (2000b).
EDTA derivatives (Inc. Tetrasodium EDTA)	57.8	57.8	500	Nowack and VanBriessen, (2005).
Fluorescent Brightener FWA-1	0.11	0.08	2.10	HERA, (2004a).
Linear Alkylbenzene Sulphonate	1030	93.7	410	IUCLID, (2000c).
Musk ketone	25.4	7.66	0.17	OSPAR Commission, (2004).
Musk xylene	11.5	1.21	0.03	EC, (2005).
N,N-Diethyl-m-toluamide (DEET)	1.57	0.14	0.01	Holloway, (2010).
Propylene glycol	54.4	3.40	4000	HSDB, (2013).
Salicylic acid	0.13	0.07	0.10	IUCLID, (2000e).
Secondary Alkane Sulphonate	1.29	0.04	1.00	HERA, (2005a).
Siloxane (D4-octamethylcyclotetrasiloxane)	0.45	0.09	0.30	IUCLID, (2000d).
Siloxane (D5-decamethyl-cyclopentasiloxane)	0.36	0.08	0.40	Health Canada, (2008a).
Siloxane (D6-dodeca-methylcyclohexasiloxane)	0.38	0.11	0.04	Health Canada, (2008b).
Triclosan	1.01	0.34	300	HSDB, (2013).
No data available for remaining compounds				

4.2.4 Drinking Water

The available data for concentrations of these PCPs and DCPs in drinking water have been summarised in Table 4.9 and compared to the modelled values. Where multiple values have been found the maximum measured occurrence value has been used. This data set is limited and there were no data available in the literature for a number of the chemicals.

The modelled estimations for benzotriazole, dimethyl phthalate, EDTA, linear alkylbenzene sulphonate and DEET all appear to be greater than measured values found in literature.

In the literature it was reported that, 2-(2-butoxyethoxy)ethanol (DEGBE), diethylene glycol ethyl ether (DEGEE), fluorescent brightener FWA-1, salicylic acid and siloxanes were detected in drinking water but the concentrations were not quantified. It can therefore be said that these chemicals have the potential to reach drinking water as shown in the literature but the concentrations at which they were detected cannot be compared to the modelled data.

The estimation for the concentration of benzophenones in drinking water is less than the measured data from literature.

Where comparisons can be made and the modelled concentrations are within a similar order of magnitude to the measured concentrations the model is not predicting concentrations that are significantly over or underestimated, especially as the predicted concentrations are averaged across the UK.

Table 4.9 Modelled concentrations in drinking water versus measured drinking water concentrations from literature

Chemical	Maximum predicted concentration in drinking water (µg/l)	Minimum predicted concentration in drinking water (µg/l)	Measured values for drinking water (µg/l)	References
1,2,3-Benzotriazole	60.0	3.77	0.79	Janna *et al*, (2011).
1H-Benzotriazole, 4(or 5)-methyl-	20.3	1.14	0.07	Janna *et al*, (2011).
2-(2-butoxyethoxy)ethanol (DEGBE)	57.4	44.1	Detected	EC, (1999).
Benzophenones	1.34	0.01	8.80	IUCLID, (2000a).
Boric acid	182	136	400	HERA, (2004a).
Dimethyl phthalate	8.34	0.60	0.27	IUCLID, (2000b).
Diethylene glycol ethyl ether (DEGEE)	172	8.82	Detected	HSDB, (2013).

Chemical	Maximum predicted concentration in drinking water (µg/l)	Minimum predicted concentration in drinking water (µg/l)	Measured values for drinking water (µg/l)	References
EDTA derivatives (Inc. Tetrasodium EDTA)	57.8	57.8	90	EC, (2004).
Fluorescent Brightener FWA-1	0.11	0.03	Detected	HSDB, (2013).
Linear Alkylbenzene Sulphonate	1030	46.8	37.0	IPCS, (1996).
N,N-Diethyl-m-toluamide (DEET)	1.57	0.08	0.012	Illanois EPA, (2008).
Salicylic acid	0.13	0.03	Detected	HSDB, (2013).
Siloxane (D4-octamethylcyclotetrasiloxane)	0.45	0.04	Detected	HSDB, (2013).
Siloxane (D5-decamethyl-cyclopentasiloxane)	0.36	0.04	Detected	Health Canada, (2008a).
Siloxane (D6-dodeca-methylcyclohexasiloxane)	0.38	0.06	Detected	Holloway, (2010).
Triclosan	1.01	0.10	0.73	HSDB, (2013).
No data available for remaining compounds				

5. Stage 3: Exposure Assessment

5.1 Exposure through Typical use

Estimates of consumer exposure to the chemicals on the prioritised list were sought from authoritative risk assessments and the wider literature. The references used in the initial data search were first examined for an estimation of the Systemic Exposure Dose (SED) resulting from exposure to these chemicals under typical use, where these values frequently took several potential routes of exposure into account (e.g. oral, dermal and inhalation). When such estimations were not located, a wider literature search was conducted, which included a search of peer-reviewed publications. Exposure estimates were taken from HERA risk assessments, Cosmetic Ingredient Review assessments, European Union Risk Assessment Reports, Health Canada risk assessments, OECD SIDS assessments, Opinions of the European Scientific Committee on Consumer Products and peer-reviewed publications. There are only four chemicals for which no quantitative exposure estimates were located; methyldibromo glutaronitrile, para-aminophenol (PAP), pentasodium pentetate and sulphamic acid. This indicates potential areas for further work. The estimates of consumer exposure SED values are listed in Table 5.5, Table 5.6 and Table 5.7. Further details of the exposure estimates located, the basis of the derivations and the references used, are located in Appendix E.

5.2 Exposure through Drinking Water

In order to compare the estimates of consumer exposure through typical use (systemic exposure doses) to the modelled concentrations in drinking water, these modelled concentrations were first converted to systemic exposure doses via both the oral and dermal routes of exposure. Exposure through inhalation of these PCPs and DCPs was not considered as part of this exposure assessment as this route was considered to be minimal to the overall exposure. The prioritisation process tends to favour those chemicals that are likely to stay within the water column and are unlikely to undergo volatilisation.

5.2.1 Oral Exposure

The systemic exposure dose arising from oral exposure to the prioritised chemicals in drinking water was estimated by assuming a 60 kg adult drinking 2 litres of water per day, and assuming 100% absorption through the gastrointestinal tract as a worst case (Table 5.1). The values of 60 kg and 2 litres are the parameters used by the World Health Organization (WHO) for deriving their Guidelines for Drinking Water Quality (GDWQ).

Table 5.1 Estimation of oral systemic exposure dose

$Exp_{sys-o} = C \times L / BW$		
Parameter	**Definition (units)**	**Assumption**
Exp_{sys-o}	Systemic exposure dose; oral (mg/kg bw/day)	-
C	Modelled concentration in drinking water (mg/l)	-
L	Drinking water consumed per day (litres)	2 litres
BW	Bodyweight (kg)	60 kg adult

5.2.2 Dermal Exposure

Exposure to chemicals in drinking water may include dermal absorption during bathing and showering. In order to estimate the dermal systemic exposure dose (Exp_{sys-d}) arising from such exposure, a simple mathematical model was utilised which combined aspects of the methodology used by the HERA risk assessments (HERA, 2002) and the US Environmental Protection Agency (EPA) for dermal risk assessment (US EPA, 2004; US EPA, 2007). This model used the concentration of the chemical in drinking water (C), the dermal penetration coefficient (Kp), the surface area of exposed skin (S_{der}) the duration of exposure (t), the frequency of tasks per day (n) and bodyweight (BW). The equation and assumptions used are shown in Table 5.2.

Table 5.2 Estimation of dermal systemic exposure dose

$Exp_{sys-d} = C \times Kp \times S_{der} \times t \times n / BW$		
Parameter	**Definition (units)**	**Assumption**
Exp_{sys-d}	Systemic exposure dose; dermal (mg/kg bw/day)	-
C	Modelled concentration in drinking water (mg/cm^3)	-
Kp	Dermal penetration coefficient (cm/h)	-
S_{der}	Surface area of exposed skin (cm^2)	Full body exposure (18 000 cm^2)
t	Duration of exposure or contact (hours)	30 minute bath (i.e. 0.5 hours)
n	Frequency (tasks per day)	1 bath per day
BW	Bodyweight (kg)	60 kg adult

The dermal penetration coefficient (Kp) used in this model of systemic exposure dose, is a measure of the rate of migration of a chemical through the skin (US EPA, 2004) and can be derived from either experimental or predicted values. In this case, experimentally determined values of Kp were used wherever these were located in the literature (see Section 5.1). However, experimental values of Kp were only located for seven chemicals (Table 5.3). Therefore, to ensure a consistent approach, Kp was estimated for the remaining chemicals using another simple model, as used by the US EPA (US EPA, 2004) and summarised in Table 5.4. In this model, Kp is estimated using a function of the octanol/water partition coefficient (Kow) and the molecular weight (MW), and this approach has been developed from an experimental database of absorption of chemicals from water through human skin *in vitro* (approximately 90 chemicals) (US EPA, 2004).

Table 5.3 Experimentally derived Kp values

Chemical name	Kp (cm/h)	Details of study	Reference
(1-hydroxyethylidene) diphosphonic acid (HEDP)	7.60E-06 a	*In vivo* dermal penetration study, using [14C]-ATMP sodium salt, in rats	HERA, (2004).
Amino tris(methylene phosphonic acid) (ATMP)			
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)			
Boric acid	1.90E-07	Skin absorption study conducted in human volunteers; 5% aqueous solution, 900 cm^2 area on the back treated for 24 hours. Boron measured in the urine.	HERA, (2005b).
Methyl paraben	6.51E-03	*In vitro* skin penetration of excised guinea pig dorsal skin	CIR, (2008).
Musk xylene	6.86E-05	*In vitro* assay conducted using hairless guinea pig skin under steady state conditions	EC, (2005).
Salicylic acid	0.0152	*In vitro* study using human epidermis from mid-abdominal skin	CIR, (2003).

a: Dermal penetration coefficient assumed to be similar for the 3 phosphonic acid compounds, on the basis of similar chemical structure and physico-chemical characteristics.

Table 5.4 Estimation of the dermal penetration coefficient (Kp)

log Kp = -2.80 + 0.66 log Kow - 0.0056 MW	
Parameter	**Definition**
Kp	Dermal penetration coefficient
Kow	Octanol/water partition coefficient
MW	Molecular weight

This model can only be used to estimate Kp for chemicals with Kow and MW within an "Effective Prediction Domain" (EPD), as determined via a statistical analysis (US EPA, 2004). In general, chemicals with very large and very small Kow values are outside the EPD. When these limits were applied to the physico-chemical parameters of the chemicals on the prioritised list, six chemicals (tetrasodium EDTA, fluorescent brightener FWA-1, pentasodium pentetate, disodium salt, and the three siloxanes) were found to be outside the EPD. However, the US EPA state that with no other data available for chemicals with very large and very small Kow, it is appropriate to use this model to derive a preliminary estimate of Kp (US EPA, 2004).

5.3 Comparison of Exposure through Drinking Water versus Exposure during typical use

5.3.1 Exposure ratios

The predicted exposure during typical use of these chemicals located in literature has been directly compared to the modelled exposure to these chemicals via drinking water and bathing in Tables 5.5 to 5.7. The ratio of the SED through typical use to exposure from drinking water and bathing for each chemical has also been reported.

Those chemicals that have a lower modelled exposure to drinking water and bathing than through their typical intended use are listed in Table 5.5. For the majority of the chemicals in this table, the exposure through drinking water and bathing is much less than the estimated exposure through intended use, ranging from 0.00009% to 0.1% of the exposure through intended use. This means the exposure from drinking water and bathing is around a thousand times less than exposure through typical use of the PCPs or DCPs. This includes some of the chemicals that had been identified in literature as having the potential to occur in drinking water such as parabens, musks siloxanes and benzophenones.

Modelled exposure estimations through drinking water and bathing water for cocamidolpropyl betaine, diethylenetriamine penta(methylene phosphonic acid) (DTPMP) and linear alkylbenzene sulphonate were lower than the exposure through typical use but the difference between the two estimated exposures was much less than the other chemicals (45%, 32%

and 84% respectively). Therefore, there is the potential for significant exposure to these chemicals through the combination of their direct, intended use, and subsequent secondary exposure from consumption of drinking water and bathing. Therefore, it may be appropriate to consider further investigation on the occurrence of these compounds in drinking water, possibly through a limited survey, and determination of the potential (if any) health implications from the predicted levels of exposure.

Seven of the original 33 chemicals modelled had estimated exposures through drinking water and bathing greater than the estimated exposure through intended use (see Table 5.6). These included amino tris(methylene phosphonic acid) (ATMP), (1-hydroxyethylidene) diphosphonic acid (HEDP), 2-(2-butoxyethoxy)ethanol (DEGBE), 1H-benzotriazole, 4(or 5)-methyl-1,2,3-benzotriazole, boric acid and EDTA derivatives (Inc. tetrasodium EDTA). Of these seven are used in domestic cleaning products five of them are used in dish and laundry cleaning. These compounds will be discussed in Section 6.

Data on the estimated exposure through typical use for four compounds could not be found (see Table 5.7). Methyldibromo glutaronitrile has been banned for use in cosmetics but it is thought that it is still used in household cleaning products and therefore may still be of concern. Para-aminophenol is used in hair dyes, and no data could be found on the exposure through this use. Data on pentasodium penetrate and sulphamic acid use in PCPs or DCPs were very limited. Further work on deriving exposure estimates would require more data on the types of PCPs and DCPs they are used in, concentrations of these chemicals in the products, the way in which the products are used, the dermal and gastrointestinal absorption rates and development of an exposure model specific to the chemical in question.

As described in Section 4.1.4, some of the assumptions applied to the model can be considered as producing an extreme “worst case” concentration in drinking water. Despite this, only seven chemicals were identified as potentially occurring in drinking water at concentrations that will result in exposure via drinking water and bathing in excess of the of that from typical use:

- Amino tris(methylene phosphonic acid) (ATMP)
- (1-Hydroxyethylidene) diphosphonic acid (HEDP)
- 2-(2-butoxyethoxy)ethanol (DEGBE)
- 1H-Benzotriazole, 4(or 5)-methyl-
- 1,2,3-Benzotriazole
- Boric acid
- EDTA derivatives (Inc. Tetrasodium EDTA)

The estimated exposure ratios for these seven chemicals are presented in Table 5.6. Therefore, exposure to twenty-six chemicals via drinking water and bathing can be concluded to be insignificant, even in the most extreme of circumstances, when compared to exposure via intended use. Refinement of the exposure assessment for these seven chemicals to reflect more realistic, but still precautionary assumptions, can be developed through the inclusion of a ten-fold dilution factor, as used in EUSES (2012).

When this dilution factor is applied to these seven chemicals, exposure via drinking water and bathing for the maximum and minimum concentrations predicted in the model are less than the exposure through normal use for amino tris(methylene phosphonic acid) (ATMP), (1-hydroxyethylidene) diphosphonic acid (HEDP) and 2-(2-butoxyethoxy)ethanol (DEGBE).

However, the exposure through drinking and water and bathing for 1H-Benzotriazole, 4(or 5)-methyl-, 1,2,3-Benzotriazole, Boric acid and EDTA derivatives (Inc. Tetrasodium EDTA) remained above the exposure through normal use for the maximum predicted concentrations (Table 5.8).

Table 5.5 Chemicals that have an estimated exposure through drinking water and bathing lower than exposure through typical use

Chemical	Exposure through typical use of PCPs and DCPs SED* (mg/kg bw/day)	Maximum exposure through drinking water and bathing water (mg/kg bw/day)	Minimum exposure through drinking water and bathing water (mg/kg bw/day)	Hazard ratio Typical use SED: exposure through potable water	
				Maximum exposure ratio	Minimum exposure ratio
Salicylic acid	0.50	0.000005	0.0000009	0.000009	0.000002
Fluorescent Brightener FWA-1	0.23	0.000004	0.000001	0.00002	0.000005
Benzophenones	1.89	0.0001	0.0000004	0.00003	0.0000002
Triethanolamine	11.4	0.0003	0.0002	0.00003	0.00001
N,N-Diethyl-m-toluamide (DEET)	1.02	0.0001	0.000003	0.00005	0.000003
Triclosan	0.57	0.00004	0.000004	0.0001	0.000007
Sodium isopropylparaben	0.59	0.00009	0.000008	0.0002	0.00001
Sodium methylparaben	0.59	0.00009	0.000003	0.0002	0.000004
Methyl paraben	0.59	0.0001	0.000002	0.0002	0.000003
Siloxane (D4-octamethylcyclotetrasiloxane)	0.24	0.00008	0.000008	0.0003	0.0000
Siloxane (D5-decamethyl-cyclopentasiloxane)	0.16	0.0002	0.00002	0.001	0.0001
Musk xylene	0.21	0.0003	0.00002	0.001	0.0001
Propylene glycol	0.72	0.0018	0.0001	0.003	0.0002
Diethylene glycol ethyl ether (DEGEE)	1.97	0.0057	0.0003	0.0029	0.00015
Siloxane (D6-dodeca-methylcyclohexasiloxane)	0.085	0.0003	0.00004	0.003	0.001
Musk ketone	0.20	0.0008	0.0001	0.004	0.0006
Bis(2-methoxyethyl) phthalate	0.009	0.0001	0.00005	0.01	0.005

Chemical	Exposure through typical use of PCPs and DCPs SED* (mg/kg bw/day)	Maximum exposure through drinking water and bathing water (mg/kg bw/day)	Minimum exposure through drinking water and bathing water (mg/kg bw/day)	Hazard ratio Typical use SED: exposure through potable water	
				Maximum exposure ratio	Minimum exposure ratio
Secondary Alkane Sulphonate	0.004	0.00004	0.000001	0.01	0.0003
Dimethyl phthalate	0.009	0.0003	0.00002	0.03	0.0022
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	0.0005	0.0001	0.00002	0.22	0.04
Cocamidopropyl betaine	0.01	0.0048	0.0	0.45	0.0
Linear Alkylbenzene Sulphonate	0.042	0.0350	0.0016	0.84	0.04

Table 5.6 Chemicals that have an estimated exposure through drinking water and bathing higher than exposure through typical use

Chemical	Exposure through typical use of PCPs and DCPs SED* (mg/kg bw/day)	Maximum exposure through drinking water and bathing water (mg/kg bw/day)	Minimum exposure through drinking water and bathing water (mg/kg bw/day)	Risk ratio Typical use SED: exposure through potable water	
				Maximum exposure ratio	Minimum exposure ratio
Amino tris(methylene phosphonic acid) (ATMP)	0.0005	0.0007	0.0002	**1.28**	0.45
(1-hydroxyethylidene) diphosphonic acid (HEDP)	0.0005	0.0007	0.0003	**1.29**	0.65
2-(2-butoxyethoxy)ethanol (DEGBE)	0.0004	0.0019	0.001	**4.46**	**3.43**
1H-Benzotriazole, 4(or 5)-methyl-	0.00002	0.0007	0.0000	**40.6**	**2.29**
1,2,3-Benzotriazole	0.00002	0.0020	0.0001	**122**	**7.64**
Boric acid	0.00004	0.0061	0.0045	**144**	**108**
EDTA derivatives (Inc. Tetrasodium EDTA)	0.00001	0.0019	0.0002	**193**	**19.0**

Table 5.7 Chemicals for which comparison between estimated exposure through drinking water and bathing and exposure through typical use cannot be made

Chemical	Exposure through typical use of PCPs and DCPs SED* (mg/kg bw/day)	Maximum exposure through drinking water and bathing water (mg/kg bw/day)	Minimum exposure through drinking water and bathing water (mg/kg bw/day)
Methyldibromo glutaronitrile	-	0.0001	0.0001
para-Aminophenol (PAP)	Negligible	0.0001	0.00004
Pentasodium pentetate	-	0.0001	0.00004
Sulphamic acid	-	0.0061	0.0061

Table 5.8 Refined exposure ratios for chemicals that have an estimated exposure through drinking water and bathing higher than exposure through typical use. (Ten-fold dilution applied)

Chemical	Exposure through typical use of PCPs and DCPs SED* (mg/kg bw/day)	Maximum exposure through drinking water and bathing water (mg/kg bw/day)	Minimum exposure through drinking water and bathing water (mg/kg bw/day)	Risk ratio Typical use SED: exposure through potable water	
				Maximum exposure ratio	Minimum exposure ratio
Amino tris(methylene phosphonic acid) (ATMP)	0.00005	0.0007	0.0002	0.13	0.05
(1-hydroxyethylidene) diphosphonic acid (HEDP)	0.00005	0.0007	0.0003	0.13	0.07
2-(2-butoxyethoxy)ethanol (DEGBE)	0.00004	0.0019	0.001	0.45	0.34
1H-Benzotriazole, 4(or 5)-methyl-	0.000002	0.0007	0.0000	4.60	0.23
1,2,3-Benzotriazole	0.000002	0.0020	0.0001	12.2	0.76
Boric acid	0.000004	0.0061	0.0045	14.4	10.8
EDTA derivatives (Inc. Tetrasodium EDTA)	0.000001	0.0019	0.0002	19.3	1.90

6. Discussion

In Stage 3 of the assessment nineteen chemicals were excluded from further assessment as they had estimated exposures during their typical intended use at much higher levels than the exposure that may be anticipated from drinking water and bathing, based on the model outputs. The remaining chemicals had estimated exposures from drinking water and bathing close to, or above, the exposure through typical use or there was not enough data with which to make an assessment.

6.1 Limitations with the model

It should be noted that the model has limitations which may explain why the exposure through drinking water and bathing is greater than the exposure through typical use of the chemicals.

The initial input concentrations are based on the UK usage estimates reported by Euromonitor. The model has assumed that 100% of the chemicals used in these products are released to the sewerage system, which is considered a pragmatic approach. This is the most precautionary assumption we can make considering a reasonable amount of the PCPs and DCPs will be released to sewerage following normal use and it is not possible to estimate how much of these products would follow different routes. It should also be noted that many of these modelled compounds have a wide range of in addition to their use in PCPs and DCPs and actual concentrations in sewage could be higher than the figures used. This assumption also does not take into account any products containing these chemicals that have been imported from outside the UK. It also assumes that these products are used equally by everyone in the UK whereas regional concentrations in influent may be higher or lower depending on the habits of the local population.

There are a large number of chemicals for which no data could be located. As such it was not possible to assess whether these chemicals are likely to occur in drinking water at any significant levels.

The removal from waste water predictions have been derived from literature and a maximum and minimum removal as reported in the literature has been used. As such, different WwTWs with different levels of treatment will achieve differing levels of treatment. It may take further work on sewage removal efficiencies for these chemicals to refine the model to determine a more accurate view of how much removal can reasonably be achieved.

The environmental partitioning section of the model assumes that there is no degradation or dilution of the chemicals in the environment and post partitioning to the soil, sediment, or air the remaining concentration in the surface water will be the raw water concentration going to drinking water treatment. These assumptions applied to the model can be considered as producing an extreme “worst case” concentration in drinking water. Despite this only seven

chemicals were identified as potentially occurring in drinking water at concentrations that will result in exposure via drinking water and bathing in excess of the of that from typical use. Therefore, refinements of the exposure assessment for these seven chemicals were developed through the inclusion of a ten-fold dilution factor as used in EUSES (2012). This dilution factor is generic and may not reflect local conditions.

The removal from drinking water has been estimated in a similar manner to that for the waste water treatment section of the model by using literature values, expert knowledge of different treatment processes and the physico-chemical properties of the chemicals.

The exposure through drinking water and bathing assessments are based on some very basic assumptions notably that exposure a 60 kg adult drinks 2 litres of water per day and that 100% of the chemical is absorbed into the body when consumed. This is consistent with the assumptions adopted by the World Health Organization (WHO) in derivation of their guidelines but may result in predictions that are an overestimate, as some chemicals may not be absorbed as readily after consumption.

Generally, this model is designed to be conservative in its estimates of the potential exposure to chemicals in drinking water that may have originated in PCPs or DCPs. Without more information on the actual concentrations reaching drinking water treatment or removal rates during drinking water treatment it is not possible to validate this assumption or assess the scale by which the model is overestimating exposure. It should also be noted that this assessment does not explore whether these chemicals are likely to be found at concentrations that are harmful to health it simply reports the potential concentrations that might be present and whether these correspond to exposures that are greater than people would normally be exposed to during typical use of the PCP or DCP products.

The chemicals that have maximum estimated exposures through drinking water or bathing close to or above the estimated exposure through typical use are discussed in the following sections.

6.2 Chelating agents

6.2.1 Phosphonates

In the original list of 692 PCP and DCP ingredients, three phosphonates were identified and all of these were within the top twenty-eight chemicals included on the prioritised list. After modelling and comparison of exposure from drinking water and bathing with exposure through typical use all three were identified as compounds that required further investigation. Amino tris(methylene phosphonic acid) (ATMP) and (1-hydroxyethylidene) diphosphonic acid (HEDP) had estimated exposures from drinking water and bathing greater than the exposure through intended use in PCPs and DCPs and diethylenetriamine penta(methylene phosphonic acid) (DTPMP) has comparable potential exposures through drinking water and bathing that appeared close to but did not exceed the exposure through typical use.

Phosphonates are chelating agents that sequester water hardness (i.e. bond with calcium and magnesium ions to prevent them interfering with the action of soaps) in dishwashing, laundry and house cleaning products. Chelating agents are very soluble, slowly biodegradable and form bonds with metals which may have implications for mobilising metals into the water column. They have been described as persistent in the environment but at low concentrations (Nowack and Van Briessen, 2005).

There were no data in the literature that suggested these compounds have been detected in drinking water. However, the results from this model suggest that they may have the potential to occur in drinking water.

6.2.2 EDTA derivatives (Inc. tetrasodium EDTA)

EDTA and its derivatives are chelating agents used in a wide range of applications including mitigation against water hardness in boilers and industrial applications, as an ingredient to sequester trace metals that cause rancidity in foods and vitamins, and to control metals that destabilise cosmetics and pharmaceuticals (Nowack and Van Briessen, 2005). It is persistent in the environment and is likely to be found at relatively high concentrations in raw waters, due to its diverse range of applications. It has been suggested that chelating agents such as EDTA may remobilise metals from sediments and soils and carry them to groundwaters and may affect the bioavailability of metals (Nowack and Van Briessen, 2005). EDTA has been banned in detergents in some countries in Europe and is restricted in detergents that are part of the voluntary ecolabel scheme run by the European Commission (EC, 2012). However, in the UK, it is used in greater quantities in personal care products than domestic cleaning products according to the data supplied by Euromonitor and so the effect of restricting EDTA in household cleaning detergents may not affect the concentrations that reach drinking water. Intake from food may be large and has not been considered in the estimates of this study.

6.2.3 Summary on chelating agents

The results from the modelling exercise and literature search indicate that there is a potential for chelating compounds, such as phosphonates and EDTA derivatives, to occur in drinking water.

Chelating compounds are used in large quantities in cosmetics, and household cleaning products such as dishwashing and laundry cleaning. However, it is reasonable to anticipate that exposure to these chemicals in such products through their intended use is limited, because products such as dishwashing tablets and laundry powders are only in contact with consumers for a short amount of time as they are transferred from the packaging to the washing machine. The systemic exposure through typical use of EDTA in cosmetics is very low due to the poor skin absorbency of EDTA. The gastrointestinal absorbencies of EDTA or phosphonates have not been included in this assessment and further research may help refine these exposure assessments or highlight if there is a health concern from oral exposure to these agents. It is beyond the scope of this assessment as to whether chelating agents

pose a toxicological risk to consumers exposed through drinking water and bathing. Though, in the case of EDTA, WHO has established a guideline value of 600 µg/l which is far in excess of the concentration estimated in this study.

6.3 Benzotriazole

Benzotriazoles were identified from the literature as having the potential to reach drinking water and had been found previously in various surface and drinking waters in the UK. During the prioritisation stage of the project 1,2,3-benzotriazole was ranked top of the prioritisation list and 1H-benzotriazole, 4(or 5)-methyl- also had a very high score compared with the other compounds on the list. Janna *et al.* (2011) reported that these benzotriazoles were identified in a number of sewage effluents in the UK at concentrations of up to 5.7 µg/l. In surface waters, Janna *et al.,* (2011) detected benzotriazoles at concentrations up to 1.2 µg/l, and it was reported that not all benzotriazole is removed during drinking water treatment by ozone or GAC. For the purposes of this assessment, exposure through use of benzotriazoles as corrosion inhibitors in dishwashing tablets was considered to be a typical source of exposure during intended use of benzotriazole-containing products. The exposure through such use would be limited, as consumers are only in contact with such tablets whilst transferring the tablet to a dishwashing machine and through small amounts of residue on the crockery and cutlery.

It should be noted that the initial usage tonnages for benzotriazoles were over-estimates as limited data could be located and the Euromonitor category used was “other miscellaneous ingredients”. However, benzotriazole has been detected in drinking waters in the UK though only at concentrations less than the maximum predicted by this model.

6.4 2-(2-Butoxyethoxy) ethanol (DEGBE)

Within the prioritised list of chemicals there were two glycol ethers 2-(2-butoxyethoxy)ethanol (DEGBE) and diethylene glycol ethyl ether (DEGEE). The estimated exposure to DEGBE through drinking water and bathing exceeded the estimated exposure through typical use. It should be noted that the influent and effluent estimates for 2-(2-butoxyethoxy)ethanol (DEGBE) are considered to be overestimates and up to 5 times higher than the measured data reported in the literature. The literature reports that DEGBE has been detected but not quantified in water supplies (no Limit of Detection (LOD) reported), which confirms the possibility of this compound reaching water supplies. The European Union risk Assessment report for DEGBE (EC, 2000) highlights that there is a general trend towards products that are water soluble and the use of DEGBE in these products will increase over time, thus increasing the risk of exposure through drinking water and bathing. Therefore, the presence of glycol ethers in drinking water could be an area that requires further assessment.

6.5 Boric acid

Boric acid is used in household cleaning products, laundry detergent, automatic dishwashing liquid and some cosmetics. It is not extensively removed during wastewater treatment and

remains in the final effluent (HERA, 2005b). Boron in the environment exists as either boric acid or boron salts. Boric acid occurs naturally in the environment and has a number of sources such as rock weathering and industrial sources. Levels of boron (as boric acid) in effluents, surface waters and drinking water have been monitored extensively and it has been reported that assessment of boric acid in any environment should take into account the natural background levels of boron (HERA, 2005b). The exposure to boric acid from drinking water and bathing did exceed the exposure through typical use of PCPs and DCPs. However, it should be noted that people are likely to be exposed to large amounts of boric acid from other sources including natural sources and therefore the significance of the level of exposure predicted by this model is uncertain. However, it should be noted that an increase in the use of boric acid in PCPs and DCPs could lead to increases in boron in drinking water above the natural background levels. Boron is a parameter under the Drinking Water Directive and any increase would be detected through routine monitoring.

6.6 Surfactants

6.6.1 Linear alkylbenzene sulphonate (LAS)

Linear alkylbenzene sulphonates (LAS) are very common anionic surfactants used in detergents. The model estimated that the maximum exposure through drinking water and bathing is slightly less than the exposure through typical use.

Between 2007 and 2012 approximately 50 000 tonnes LAS has been used in the UK annually in PCPs and DCPs. This was the highest tonnage chemical listed in the Euromonitor database of PCP and DCP chemicals. When this value was converted to a concentration in treatment works influent it equated to 10 956 µg/l (approximately 11 mg/l). This input to the wastewater treatment works was by far the largest contribution of all the chemicals on the prioritised list. LAS is reported to be readily biodegradable and the model reflects this with a 99% maximum removal rate from wastewater treatment. However, this means that 1% of the initial concentration goes to the surface waters which equates to about 100 µg/l. A review of occurrence data in the literature indicated that concentrations in effluent from wastewater treatment works have reached 273 µg/l, in surface waters LAS concentrations of up to 410 µg/l were reported, and in drinking water concentrations of 37 µg/l were reported (see Section 4.2). This shows that despite LAS being biodegradable it is used in such high quantities that it still has the potential to occur in drinking water supplies.

6.6.2 Cocamidopropyl betaine

Cocamidopropyl betaine is an amphoteric surfactant used in cosmetics such as shampoos and hand soap as a foam booster. The maximum estimated exposure through drinking water and bathing is about half of the estimated exposure through typical use. The initial concentrations entering the wastewater treatment works are likely to be overestimates. The category provided by Euromonitor was “alkyl amido alkyl betaines” which will contain data for other similar compounds. The removal during wastewater treatment ranged between 90% removal and 100% which suggests a high level of removal. It is thought that the actual

concentrations of cocamidopropyl betaine will be less than estimated for this assessment and the high level of removal will decrease the amount of exposure through drinking water and bathing further.

6.6.3 Summary on surfactants

Surfactants such as LAS and cocamidopropyl betaine are used in large quantities in detergents used in PCPs and DCPs. There is legislation which limits the use of non-biodegradable surfactants[2], which aims to protect the environment from these substances. However, total degradation cannot be guaranteed and with high expected volumes of these surfactants in influents there is a possibility for these substances to reach drinking water.

In the UK between 1995 – 2003, 22 978 drinking water samples were taken and 10 samples exceeded the Prescribed Concentration Value (PCV) of 200 µg/l for surfactants (as lauryl sulphate) under The Water Supply (Water Quality) Regulations 1989. Between 2009 and 2013, 4118 samples raw water were taken, and 64 samples had concentrations of surfactants above 200 µg/l. Current drinking water legislation in the UK does not have a drinking water standard for surfactants. These data indicate that surfactants very rarely reach drinking water at concentrations above the former PCV.

6.7 Overall summary

Of the thirty-three modelled chemicals nineteen were predicted to have maximum exposures through drinking water and bathing that were much lower than exposure through typical use. These were excluded from further consideration. Ten of the modelled compounds were found to have estimated maximum exposures through drinking water and bathing that were close to, or exceeded, the exposure through typical use. Four of these were chelating agents such as phosphonates and EDTA and its derivatives. There is evidence from the literature that chelating agents such as these have reached drinking water supplies. The main use of chelating agents is to sequester water hardness and metals that will interfere with the action of the detergents. Benzotriazoles, which are used as corrosion inhibitors in dishwashing applications, were identified as compounds of interest in the initial data search and they also came very high in the prioritisation exercise. However, the initial concentrations of these compounds going to wastewater treatment may be overestimated. 2-(2-butoxyethoxy)ethanol (DEGBE) is a glycol ether that may be increasingly used in the future to make products water soluble. It has already been detected in drinking water supplies and increases in usage may have implications for drinking water quality over time. Surfactants such as linear alkylbenzene sulphonate and cocamidopropyl betaine are used in huge quantities in PCPs and DCPs. Despite the requirement that surfactants are biodegradable there is still potential for these compounds to reach drinking water as has been shown in literature.

[2] Regulation (EC) No 648/2004 of the European Parliament and of the Council of 31 March 2004 on detergents.

Further refinement of the model involved applying a ten-fold dilution factor to the concentrations in the environment. This resulted in the exposure via drinking water and bathing dropping below the exposure through normal use for three compounds (amino tris(methylene phosphonic acid) (ATMP), (1-hydroxyethylidene) diphosphonic acid (HEDP) and 2-(2-butoxyethoxy)ethanol (DEGBE)). However, the exposure through drinking and water and bathing for 1H-Benzotriazole, 4(or 5)-methyl-, 1,2,3-Benzotriazole, Boric acid and EDTA derivatives (Inc. Tetrasodium EDTA) remained above the exposure through normal use for the maximum predicted concentrations.

6.8 Conclusions

This study aimed to investigate the potential for ingredients used in personal care products (PCPs) and domestic cleaning products (DCPs) to reach finished drinking water. It also intended to assess whether people could potentially be exposed to these ingredients at higher amounts from drinking water and bathing than through typical use of the PCPs and DCPs.

A three staged exposure assessment was devised in order to assess the potential for people to be exposed to these chemicals via drinking water.

Stage 1: a list of 692 chemicals ingredients from a range of PCPs and DCPs was developed. The chemicals on this list then underwent a prioritisation process by which chemicals with a higher potential for reaching drinking water were identified. From this process of prioritisation thirty-three chemicals were identified to be investigated further.

Stage 2: the thirty-three identified chemicals in the prioritisation stage were modelled for their potential to reach drinking water. It was assumed that the total volume of the chemical that is used in PCPs or DCPs within the UK enters the sewerage system and potential influent concentrations were estimated from this assumption. The removal during wastewater treatment was estimated and the potential effluent concentrations going to surface water were derived. Fugacity modelling was used to estimate the amount of each chemical would partition to sediment, water or air in the environment and so estimate raw water concentrations going to drinking water treatment. This was estimated assuming that there is no dilution or degradation in the environment. The structure and physico-chemical properties of each chemical were then used to estimate the level of potential removal during different levels of drinking water treatment. The final concentration represents the potential concentrations in drinking water.

The estimated concentrations of each chemical at various stages of the model were compared to measured concentrations located in literature where these were available. The measured concentration datasets were limited and no data on measured concentrations were located for some chemicals. This comparison suggested that the model had overestimated concentrations of some of the compounds in drinking water. There were also, a few compounds that had modelled concentrations lower than those reported in the literature. It should be noted that there may be sources of these chemicals in drinking water other than

from the use of PCPs and DCPs, as many of the chemicals are used for other applications. It is also possible that the measured concentrations in literature were measured in response to a specific contamination event. Where comparisons can be made, the modelled concentrations are within a similar order of magnitude to the measured concentrations.

Stage 3: the final drinking water concentrations were used, alongside supplemental data, to estimate the potential daily exposure to these chemicals through drinking water and bathing. This value was compared to estimated exposure through typical use taken from published authoritative risk assessments. Of the thirty-three chemicals modelled, nineteen had estimated exposures from drinking water and bathing that were significantly lower than exposure through typical use of PCPs and DCPs. Ten of the thirty-three modelled chemicals had estimated exposures through drinking water and bathing that were greater than or close to the estimated exposure through typical use of PCPs and DCPs. Four of the chemicals could not be compared as no authoritative exposure assessments for typical use were located.

The ten chemicals that have maximum estimated exposures through drinking water and bathing higher than or close to the estimated exposure through typical use are:

- Chelating agents
  - Phosphonates (HEDP, ATMP, DTPMP)
  - EDTA (including its derivatives)
- Benzotriazoles
  - 1,2,3-benzotriazole
  - 1H-benzotriazole, 4(or 5)-methyl-
- 2-(2-butoxyethoxy)ethanol (DEGBE)
- Boric Acid
- Surfactants
  - Linear alkylbenzene sulphonate (LAS)
  - Cocamidopropyl betaine

The inclusion of a dilution factor to refine this model would mean that the exposure through drinking water and bathing could decrease below the exposure through normal use for three of these compounds, however a suitable dilution factor would need to be derived for the UK that would suitably reflect local conditions.

This study has not identified whether these chemicals could be of toxicological concern in drinking water but has provided a high level screen for the vast number of chemicals that are being used every day in PCPs and DCPs and provided a shortlist of chemicals that have the potential to reach drinking water supplies.

7. Areas of Further Research

This project has shown that there may be a risk that a number of constituents of PCP and DCP could reach drinking water supplies. It has screened a large number of chemicals and estimated that a few are more likely to occur in drinking water than others. These chemicals could be used for any further targeted assessment of drinking water in the UK.

Further work on the exposure assessments through typical use of the four chemicals that did not have authoritative exposure assessments would require more data on the types of PCPs and DCPs they are used in, concentrations of these chemicals in the products, the way in which the products are used, the dermal and gastrointestinal absorption rates and development of an exposure model specific to the chemical in question.

There is relatively little data on the occurrence of these chemicals in drinking water in the UK. The following data requirements would be beneficial to assess the impact of these PCPs and DCPs on drinking water within the UK:

- identification of when and where concentrations of PCP and DCP compounds will be highest;
- targeted monitoring at these locations at specific times of year, e.g. downstream of WwTW on highly reused rivers during dry winter periods when biodegradation would be slow and river flows would be average; and
- targeted monitoring of drinking water supplies across the UK to identify the extent of any occurrence of these compounds in drinking water in the UK.

The data on the removal efficiencies of waste water treatment and drinking water treatment processes could be improved through testing and monitoring. This could be used to refine the model to give a better estimate of actual concentrations reaching drinking water.

This project has not assessed whether these chemicals are of toxicological concern to people ingesting them via drinking water or being exposed to them dermally during bathing. Further information on the toxicological properties for those chemicals that appear to have the highest potential to reach drinking water supplies could help inform monitoring programmes.

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Appendix B Initial Chemical List

Table B.1 List of chemicals taken to prioritisation and their prioritisation score

Chemical name (common)	CAS number	Main category	Prioritisation Score
1,2,3-Benzotriazole	95-14-7	Benzotriazole	42
1H-Benzotriazole, 4(or 5)-methyl-	29385-43-1	Benzotriazole	38
Boric acid	10043-35-3	Enzyme stabiliser	38
EDTA	6381-92-6	Chelating	38
(1-hydroxyethylidene) diphosphonic acid (HEDP)	2809-21-4	Phosphonate	37
Amino tris(methylene phosphonic acid) (ATMP)	6419-19-8	Phosphonate	37
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	15827-60-8	Phosphonate	37
pentasodium pentetate	140-01-2	Chelating	37
sodium bicarbonate	144-55-8	Buffering agent	37
sodium sulphate	7757-82-6	Bulking agent	37
Tetrasodium EDTA	64-02-8	Chelating	37
2-(2-butoxyethoxy)ethanol (DEGBE)	112-34-5	Solvent	36
Methyldibromo glutaronitrile	35691-65-7	Preservative	36
Secondary Alkane Sulfonate	68037-49-0	Anionic surfactant	36
Silicic acid, disodium salt (anhydrous)	6834-92-0	Buffering agent	36
Sodium chloride	7647-14-5	Bulking agent	36
Sulfamic acid	5329-14-6	Buffering agent	36
Benzenesulphonic acid, C10-13 alkyl derivs., sodium salts	68411-30-3	Anionic surfactant	35
Citric acid	77-92-9; 5949-29-1; 6132-04-3	Buffering agent	35
Cocamidopropyl betaine (cosmetic grade)	61789-40-0, 83138-08-3, 86438-79-1	Amphoteric surfactant	35
Cocamidopropyl betaine (technical grade)	4292-10-8	Amphoteric surfactant	35
Dimethyl phthalate	131-11-3	Phthalate	35
Ethoxydiglycol	111-90-0	Humectant	35
Fluorescent Brightener FWA-1	16090-02-1	Fluorescent whitening agent	35
para-Aminophenol	123-30-8, 51-78-5	Hair dye	35
Propylene glycol	57-55-6	Humectant	35
Salicylic acid	69-72-7	Conditioning agent	35
Triethanolamine	102-71-6	Buffering agent	35
4-amino-2-hydroxytoluene	2835-95-2	Hair dye	34
4-Aminobenzoic acid	150-13-0	UV-filter	34
5-hydroxy-2-hydroxymethyl-4-pyrone	501-30-4	Preservative	34
Acetone	67-64-1	Solvent	34
Allantoin	97-59-6	Conditioning agent	34
Ammonium hydroxide	1336-21-6	Buffering agent	34
Benzoic acid	65-85-0	Preservative	34
Benzophenone-4	4065-45-6	UV-filter	34
Benzyl alcohol	100-51-6	Solvent	34
Bis(2-methoxyethyl) phthalate	117-82-8	Phthalate	34
Calcium carbonate	471-34-1	Bulking agent	34

Chemical name (common)	CAS number	Main category	Prioritisation Score
Disodium distyrylbiphenyl disulfonate	27344-41-8	Fluorescent whitening agent	34
Erythobic acid	89-65-6	Oxidising	34
Glycol salicylate	87-28-5	UV-filter	34
m-Aminophenol	591-27-5	Hair dye	34
Methylparaben	99-76-3	Paraben	34
Panthenol	81-13-0	Conditioning agent	34
Phosphoric acid	7664-38-2	Buffering agent	34
Polycarboxylates	9003-01-4, 52255-49-9	Emulsifier	34
Potassium carbonate	584-08-7	Buffering agent	34
P-Phenylenediamine	106-50-3	Hair dye	34
Sodium carbonate	497-19-8, 5968-11-6	Water softener	34
Sodium dodecylbenzenesulphonate	25155-30-0	Anionic surfactant	34
Sodium isopropylparaben	35285-69-9	Paraben	34
Sodium methylparaben	5026-62-0	Paraben	34
Sodium percarbonate	15630-89-4	Bleaching agent	34
Toluene-2,5-diamine	95-70-5	Hair dye	34
Trisodium EDTA	150-38-9	Chelating	34
1-(ß-hydroxyethyl)amino-2-nitro-4-N-ethyl-N-(ß-hydroxyethyl) aminobenzene (hydrochloride)	132885-85-9	Hair dye	33
1,2,4-Trihydroxybenzene	533-73-3	Hair dye	33
1,3-Bis-(2,4-diaminophenoxy)propane (tetrahydrochloride)	74918-21-1(tetrahydrochloride)	Hair dye	33
1-[(2'-methoxyethyl)amino]-2-nitro-4-[di-(2'-hydroxyethyl)amino]benzene	23920-15-2	Hair dye	33
1-Amino-5-chloro-4-(2,3-dihydroxypropyl)amino-2-nitrobenzene	95576-89-9	Hair dye	33
1-chloro-2,5-di((2,3-dihyroxypropyl)amino)-4-nitrobenzene	95576-92-4	Hair dye	33
1-γ-Hydroxypropylamino-2-nitro-4-bis-(ß-hydroxyethylamino)-benzene	104226-19-9	Hair dye	33
2,4,5,6-Tetraaminopyrimidine sulphate	5392-28-9	Hair dye	33
2,5,6-Triamino-4-pyrimidinol sulphate	1603-02-7	Hair dye	33
2,7-Naphthalenediol	582-17-2	Hair dye	33
2-Amino-3-hydroxypyridine	16867-03-1	Hair dye	33
2-amino-4-hydroxyethylaminoanisole sulphate (sulphate)	83763-48-8	Hair dye	33
2-butoxyethanol or ethylene glycol monobutyl ether	111-76-2	Solvent	33
2-Methyl-5-hydroxyethylaminophenol	55302-96-0	Hair dye	33
2-Nitro-5-glyceryl methylaniline	80062-31-3	Hair dye	33
3-amino-2,4-dichlorophenol HCL (Hydrochloride)	61693-43-4	Hair dye	33
3-nitro-p-hydroxyethylaminophenol	65235-31-6	Hair dye	33
4-Amino-m-cresol	2835-99-6	Hair dye	33
4-hydroxyphenyl-β-glucopyranoside, INCI name Arbutin	497-76-7	Skin lightener	33
4-hydroxypropylamino-3-nitrophenol	92952-81-3	Hair dye	33
5-Amino-4-hydroxy-3-phenylazo-2,7-naphthalenedisulfonic acid	3567-66-6	Hair dye	33
6-hydroxyindole	2380-86-1	Hair dye	33
6-methoxy-2-methylamino-3-aminopyridine HCl	83732-72-3	Hair dye	33

Chemical name (common)	CAS number	Main category	Prioritisation Score
8-[(4-Aminophenyl)diazenyl]-7-hydroxy-N,N,N-trimethylnaphthalen-2-aminium chloride	26381-41-9	Hair dye	33
Acid Yellow 1	846-70-8	Hair dye	33
Alcohol ethoxylates Ceteth-30	9004-95-9	Non-ionic surfactant	33
Alcohol ethoxylates laureth-23 C12	9002-92-0	Non-ionic surfactant	33
Ammonium thioglycolate	5421-46-5	Conditioning agent	33
Borax	1303-96-4	Enzyme stabiliser	33
Butylene glycol	107-88-0	Humectant	33
Camphor	76-22-2	Plasticiser	33
Camphor benzalkonium methosulphate	52793-97-2	UV-filter	33
Coumarin	91-64-5	Fragrance	33
Cyclomusk	29171-20-8, 5663-88-7	Musks	33
Dihydroxyindole	3131-52-0	Hair dye	33
Dipropylene glycol	25265-71-8	Humectant	33
Disodium EDTA	139-33-3	Chelating	33
Ethanolamine	141-43-5	Buffering agent	33
Ethylene glycol	107-21-1	Phthalate	33
Ethylparaben	120-47-8	Paraben	33
Hema	868-77-9	Film forming	33
Hexylene glycol	107-41-5	Emulsifier	33
Hydrogen peroxide	7722-84-1	Bleaching agent	33
Hydroxyanthraquinone-aminopropyl methyl morpholinium methosulphate	38866-20-5	Hair dye	33
Hydroxybenzomorpholine	26021-57-8, 977067-94-9	Hair dye	33
Hydroxyethyl-3,4-methylenedioxyaniline hydrochloride	94158-14-2	Hair dye	33
Hydroxyethyl-p-phenylenediamine sulphate	93841-25-9	Hair dye	33
Hydroxypropyl bis(N-hydroxyethyl-p-phenylenediamine) hcl	128729-28-2	Hair dye	33
Icaridin	119515-38-7	Insect repellants	33
IR3535	52304-36-6	Insect repellants	33
Isatin	91-56-5	Hair dye	33
Isopropylparaben	4191-73-5	Paraben	33
N1,N4,N4-Tris-(2-hydroxyethyl)-1,4-diamino-2-nitrobenzene	33229-34-4	Hair dye	33
Nitrocellulose	9004-70-0	Film forming	33
N-Phenyl-p-phenylenediamine	101-54-2	Hair dye	33
Perboric acid, sodium salt, tetrahydrate	10486-00-7	Bleaching agent	33
phenyl methyl pyrazolone	89-25-8	Hair dye	33
Phenylbenzimidazole sulfonic acid	27503-81-7	UV-filter	33
p-Methylaminophenol sulphate	1936-57-8	Hair dye	33
Potassium biphthalate	877-24-7	Phthalate	33
Propylparaben	94-13-3	Paraben	33
Silicic acid, disodium salt (crystalline pentahydrate)	10213-79-3	Buffering agent	33
Silicic acid, sodium salt	1344-09-8	Buffering agent	33
Sodium cumenesulfonate	32073-22-6, 28348-53-0	Hydrotrope	33
Sodium fluoride	7681-49-4	Oral care	33
Sodium lauryl sulphate	151-21-3	Anionic surfactant	33
Sodium tripolyphosphate	7758-29-4	Bulking agent	33
Sorbitol	50-70-4	Humectant	33

Chemical name (common)	CAS number	Main category	Prioritisation Score
Toluene-2,5-diamine (sulphate)	615-50-9, 6369-59-1	Hair dye	33
Zeolite A P and X	1318-02-1, 1344-00-9	Bulking agent	33
1-(ß-aminoethylamino)-4-(ßhydroxyethyloxy)-2-nitrobenzene	85765-48-6	Hair dye	32
1-naphthol	90-15-3	Hair dye	32
2-amino-4-hydroxyethylaminoanisole sulphate (free base)	83763-47-7	Hair dye	32
3-amino-2,4-dichlorophenol HCL (free base)	61693-42-3	Hair dye	32
4-amino-3-nitrophenol	610-81-1	Hair dye	32
4-Nitro-o-phenylenediamine (free base)	99-56-9	Hair dye	32
Acetaminosalol	118-57-0	UV-filter	32
Ascorbic acid	50-81-7	Buffering agent	32
Benzophenone-1	131-56-6	UV-filter	32
Benzophenone-2	131-55-5	UV-filter	32
Butyl acetate	123-86-4	Solvent	32
Cetrimonium chloride	112-02-7	Preservative	32
DEET	134-62-3	Insect repellants	32
Diethyl phthalate	84-66-2	Phthalate	32
Diethylene glycol	111-46-6	Solvent	32
Dihydroxyacetone	96-26-4	Conditioning agent	32
Diisopropyl adipate	6938-94-9	Emollient	32
Fluorescent brightener 230	27344-06-5	Fluorescent whitening agent	32
Formic acid	64-18-6	Preservative	32
Glycerin	56-81-5	Humectant	32
Glycol HEMA-Methaacrylate	97-90-5	Film forming	32
Quinolinium, 4-formyl-1-methyl-, salt with 4-methylbenzenesulfonic acid	223398-02-5	Hair dye	32
Sodium benzoate	532-32-1	Preservative	32
Tetraacetylethylenediamine (TAED)	10543-57-4	Bleaching agent	32
Toluene sulfonate, sodium salt	12068-03-0	Hydrotrope	32
Xylene sulfonate, sodium salt	827-21-4, 1300-72-7	Hydrotrope	32
Zinc chloride	7646-85-7	Oral care	32
Zinc stearate	557-05-1	Anticaking	32
1,5-Di-(ß-hydroxyethylamino)-2-nitro-4-chlorobenzene	109023-83-8	Hair dye	31
1,5-naphthalenediol	83-56-7	Hair dye	31
1-Hydroxyethyl-4,5-diamino pyrazole sulphate	155601-30-2	Hair dye	31
2,2'-[(4-Amino-3-nitrophenyl)imino]-bisethanol hydrochloride (hydrochloride)	94158-13-1	Hair dye	31
2,4-Diaminophenoxyethanol (Dihydrochloride)	66422-95-5	Hair dye	31
2,6-Dihydroxy-3,4-dimethylpyridine	84540-47-6	Hair dye	31
2,6-Dimethoxy-3,5-pyridinediamine dihydrochloride	56216-28-5	Hair dye	31
2-Amino-6-chloro-4-nitrophenol	6358-09-4	Hair dye	31
2-chloro-6-ethylamino-4-nitrophenol	131657-78-8	Hair dye	31
2-hydroxyethyl picramic acid	99610-72-7	Hair dye	31
2-hydroxyethylamino-5-nitroanisole	66095-81-6	Hair dye	31
2-methylresorcinol	608-25-3	Hair dye	31
4-Nitrophenyl aminoethylurea	27080-42-8	Hair dye	31
Acid Violet 43	4430-18-6	Hair dye	31
Ammonium persulphate	7727-54-0	Bleaching agent	31
Basic Brown 17	68391-32-2	Hair dye	31

Chemical name (common)	CAS number	Main category	Prioritisation Score
Benzalphthalide	575-61-1	UV-filter	31
Butylparaben	94-26-8	Paraben	31
Choline chloride	67-48-1	Humectant	31
Cinoxate	104-28-9	UV-filter	31
Drometrizole	2440-22-4	UV-filter	31
Ethanol	64-17-5	Antimicrobial	31
Ethyl cinnamate	103-36-6	UV-filter	31
Ethyl lauroyl arginate hcl	60372-77-2	Cationic surfactants	31
Glyoxal	107-22-2	Used in production of other compounds	31
Hydrogen-3,6-bis(diethylamino)-9-(2,4-disulphonatophenyl)xanthylium	3520-42-1	Hair dye	31
Hydroxyethyl-2-nitro-p-toluidine	100418-33-5	Hair dye	31
Isobutylparaben	4247-02-3	Paraben	31
Isopropyl alcohol	67-63-0	Solvent	31
Laureth-9	3055-99-0	Non-ionic surfactant	31
N,N-bis(2-hydroxyethyl)-p-phenylenediamine sulphate	54381-16-7	Hair dye	31
PEG-4 Dimethacrylate	109-17-1	Builder	31
Potassium persulphate	7727-21-1	Bleaching agent	31
Protease	9001-92-7	Detergent enzymes	31
sec-butyl acetate	105-46-4	Solvent	31
Silicic acid, disodium salt (crystalline nonahydrate)	13517-24-3	Buffering agent	31
Silicic acid, potassium salt	1312-76-1	Buffering agent	31
Sodium hydroxide	1310-73-2	Buffering agent	31
Sodium laureth sulphate	9004-82-4	Anionic surfactant	31
Sodium persulphate	7775-27-1	Bleaching agent	31
triclosan	3380-34-5	Antimicrobial	31
Xylene sulfonate, ammonium salt	26447-10-9	Hydrotrope	31
1-Amino-3-methyl-4(2-hydroxyethyl)-amino-6-nitrobenzene	82576-75-8	Hair dye	30
3-methylamino-4-nitrophenoxyethanol	59820-63-2	Hair dye	30
4-Nitro-o-phenylenediamine (Dihydrochloride)	6219-77-8	Hair dye	30
4-Nitro-o-phenylenediamine (sulphate)	68239-82-7	Hair dye	30
5-Amino-4-chloro-o-cresol hydrochloride	110102-85-7	Hair dye	30
Acid Violet 44	4430-18-7	Hair dye	30
Amylase	9000-90-2	Detergent enzymes	30
Basic Orange 69	226940-14-3	Hair dye	30
Benzophenone	119-61-9	UV-filter	30
Benzophenone-10	1641-17-4	UV-filter	30
Benzophenone-3	131-57-7	UV-filter	30
Benzophenone-6	131-54-4	UV-filter	30
Benzophenone-8	131-53-3	UV-filter	30
Benzyl salicylate	118-58-1	UV-filter	30
Cellulase	9012-54-8	Detergent enzymes	30
Di-isobutyl phthalate (DIBP)	84-69-5	Phthalate	30
Fatty acid salts C12	Fatty Acid (See Group_Fatty Acids tab)	Anionic surfactant	30
Hydrochloric acid	7647-01-0	Buffering agent	30

Chemical name (common)	CAS number	Main category	Prioritisation Score
Hydroxycitronellal	107-75-5	Fragrance	30
Indocyanine green	3599-32-4	UV-filter	30
Lauramide DEA	120-40-1	Surfactant	30
Lipase	9001-62-1	Detergent enzymes	30
Methyl salicylate	119-36-8	Fragrance	30
Optical brightners	No CAS	Fluorescent whitening agent	30
PEG-100 Stearate	9004-99-3	Surfactant	30
Perboric acid, sodium salt, monohydrate	10332-33-9	Bleaching agent	30
Propylene glycol n-butyl ether	5131-66-8 , 29387-86-8	Solvent	30
Resorcinol	108-46-3	Hair dye	30
Ricinus communis (Castor) seed oil	8001-79-4	Emollient	30
Sodium butylparaben	36457-20-2	Paraben	30
Sodium ethylparaben	35285-68-8	Paraben	30
Toluene	108-88-3	Solvent	30
2,2'-methylenebis-4-aminophenol HCl	27311-52-0	Hair dye	29
2-Nitro-4-aminodiphenylamine	2784-89-6	Hair dye	29
3-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene carbaldehyde	51414-25-6	Fragrance	29
3-benzylidene camphor	15087-24-8	UV-filter	29
4-methylbenzylidene camphor	36861-47-9 , 38102-62-4	UV-filter	29
Acid blue 62	4368-56-3	Hair dye	29
AHTN-Polycyclic musk	1506-02-1	Chelating	29
Alcohol ethoxylates C10	No CAS	Non-ionic surfactant	29
Alcohol ethoxysulphate C12	No CAS	Anionic surfactant	29
Alcohol ethoxysulphate C13	No CAS	Anionic surfactant	29
Alcohol ethoxysulphate C14	No CAS	Anionic surfactant	29
allyl 2-methylbutoxyacetate	67634-01-9	Fragrance	29
Allyl 3,5,5-trimethylhexanoate	71500-37-3	Fragrance	29
Allyl butyrate	2051-78-7	Fragrance	29
Allyl cinnamate	1866-31-5	Fragrance	29
Allyl cyclohexaneacetate	4728-82-9	Fragrance	29
Allyl cyclohexanepropionate	2705-87-5	Fragrance	29
Allyl cyclohexyloxyacetate	68901-15-5	Fragrance	29
Allyl hexanoate	123-68-2	Fragrance	29
Allyl isoamyloxyacetate	67634-00-8	Fragrance	29
Allyl isovalerate	2835-39-4	Fragrance	29
Allyl nonanoate	7493-72-3	Fragrance	29
Allyl octanoate	4230-97-1	Fragrance	29
Allyl phenoxyacetate	7493-74-5	Fragrance	29
Allyl phenylacetate	1797-74-6	Fragrance	29
Allyl propionate	2408-20-0	Fragrance	29
Allyl trimethylhexanoate	68132-80-9	Fragrance	29
Ambrettolide	7779-50-2	Musks	29
Aminomethyl propanol	68298-05-5	Buffering agent	29
Amodimethicone	71750-80-6	Conditioning agent	29
Angelica archangelica L.	8015-64-3	Fragrance	29
Bees wax	8012-89-3	Emollient	29
Behentrimonium chloride	17301-53-0	Preservative	29
Benzophenone-5	6628-37-1	UV-filter	29
Bergamot oil	8007-75-8	Fragrance	29
Bisabolol/levomenol	23089-26-1	Conditioning agent	29

Chemical name (common)	CAS number	Main category	Prioritisation Score
Bumetrizole	3896-11-5	UV-filter	29
Butane	106-97-8	Propellant	29
Camellia sinensis leaf extract	84650-60-2	UV-filter	29
Carthamus tinctorius (safflower) seed oil	8001-23-8	Conditioning agent	29
Cellulose gum	9004-32-4	Film forming	29
Citrus aurantium L.	68916-04-1	Fragrance	29
Citrus paradisi Macf.	8016-20-4	Fragrance	29
Copernicia cerifera (carnauba) wax	8015-86-9	Emollient	29
Cresylpropionaldehyde	5406-12 2	Fragrance	29
Dibutyl phthalate	84-74-2	Phthalate	29
Dicalcium phosphate dihydrate	7789-77-7	Oral care	29
Dimethicone	9006-65-9	Conditioning agent	29
Disodium cocoamphodiacetate	68650-39-5	Surfactant	29
Eucalyptus citriodora oil	8000-48-4	Insect repellants	29
Fatty acid salts C10	Fatty Acid (See Group_Fatty Acids tab)	Anionic surfactant	29
Helvetolide	141773-73-1	Musks	29
Hibiscus abelmoschus extract/oil	84455-19-6	Musks	29
Hydrated silica	112926-00-8	Abrasive	29
Isobutane	75-28-5	Propellant	29
Isodecylparaben	2664-60-0	Paraben	29
Kaolin	1332-58-7	Abrasive	29
L. orientalis	94891-27-7	Fragrance	29
L. styraciflua	8046-19-3	Fragrance	29
Lawsonia inermis (Henna)	84988-66-9	Hair dye	29
Lecithin	8002-43-5	Emollient	29
Lemon oil	8008-56-8	Fragrance	29
Lime oil	8008-26-2	Fragrance	29
Magnesium silicate	1343-88-0	Bulking agent	29
m-Aminophenol (Sulphate 2:1)	68239-81-6	Hair dye	29
Mannanase	37288-54-3	Detergent enzymes	29
Mentha piperita (peppermint) oil	84082-70-2	Fragrance	29
Menthanediol	42822-86-6	Insect repellants	29
Menthyl anthranilate	134-09-8	UV-filter	29
Methyl-n-methylanthranilate	85-91-6	Fragrance	29
Musk acetate	25225-10-9	Musks	29
Musk indanone	33704-61-9	Musks	29
Musk ketone	81-14-1	Musks	29
Musk xylene	81-15-2	Musks	29
Nonoxynol-2	27176-93-8	Surfactant	29
Nonoxynol-9	26571-11-9	Surfactant	29
Oak moss	9000-50-4	Fragrance	29
Octrizole	3147-75-9	UV-filter	29
Octyl dodecanol	5333-42-6	Emollient	29
Opopanax	93686-00-1	Fragrance	29
para-Aminophenol (hydrochloride)	51-78-5	Fragrance	29
Paraffin	8002-74-2	Emollient	29
PEG-2 cocamine	61791-14-8	Emulsifier	29
PEG-30 hydrogenated castor oil	61788-85-0	Surfactant	29
PEG-32	25322-68-3	Humectant	29
PEG-6 laurate	9004-81-3	Emulsifier	29
Perboric acid, sodium salt, mono and tetrahydrate	11138-47-9	Bleaching agent	29

Chemical name (common)	CAS number	Main category	Prioritisation Score
Perboric acid, sodium salt, mono and tetrahydrate	11138-47-9	Bleaching agent	29
Perboric acid, sodium salt, monohydrate	10332-33-9	Bleaching agent	29
Perboric acid, sodium salt, tetrahydrate	10486-00-7	Bleaching agent	29
Peru balsam	8007-00-9	Fragrance	29
Phenyl trimethicone	2116-84-9	Conditioning agent	29
Phenylparaben	17696-62-7	Paraben	29
Pinus pinaster bark/bud extract	90082-75-0	UV-filter	29
Poloxamer 184	9003-11-6	Surfactant	29
Polybutylene terephthalate	26062-94-2	Phthalate	29
Polyquaternium-10	68610-92-4	Film forming	29
Polysilicone-15	207574-74-1	UV-filter	29
Polysorbate 20	9005-64-5	Surfactant	29
Potassium alum	10043-67-1, 7784-24-9	Astringent	29
Potassium hydroxide	1310-58-3	Buffering agent	29
PPG-15	25322-69-4	Conditioning agent	29
Quaternium-95	1030827-59-8	UV-filter	29
Silica	63231-67-4	Bulking agent	29
Siloxane D5 (decamethylcyclopentasiloxane)	541-02-6	Siloxanes	29
Sodium acrylates copolymer	7446-81-3	Viscosity control	29
Sodium metaphosphate	10361-03-2	Buffering agent	29
Sodium paraben	114-63-6, 85080-04-2		29
Sodium phosphate	7632-05-5	Buffering agent	29
Starch	9005-25-8	Abrasive	29
Steartrimonium chloride	112-03-8	Preservative	29
T. erecta Flower Extract	90131-43-4	Fragrance	29
T. minuta Flower Extract	91770-75-1	Fragrance	29
T. patula Flower Extract	91722-29-1	Fragrance	29
Talc	14807-96-6	Bulking agent	29
T-butyl benzoyl peroxide	614-45-9	UV-filter	29
Tea-salicylate	2174-16-5	UV-filter	29
TEA-stearate	4568-28-9	Surfactant	29
Tree moss	68648-41-9	Fragrance	29
Tris(tetramethylhydroxypiperidinol) citrate	220410-74-2	UV-filter	29
Verbena	8024-12 2	Fragrance	29
Vetiveryl acetate	62563-80-8	Fragrance	29
Xanthan gum	11138-66-2	Surfactant	29
Zinc ricinoleate	13040-19-2	Deodorant	29
1-(ß-hydroxyethyl)amino-2-nitro-4-N-ethyl-N-(ß-hydroxyethyl) aminobenzene (free base)	104576-93-0	Hair dye	28
1-(3,4-dimethoxyphenyl)-4,4-dimethyl-1,3-pentanedione (JPN)	135099-97-7	UV-filter	28
1,3-Bis-(2,4-diaminophenoxy)propane (free base)	81892-72-0 (free base)	Hair dye	28
2,2'-[(4-Amino-3-nitrophenyl)imino]-bisethanol hydrochloride (free base)	29705-39-3	Hair dye	28
2,4-Diaminophenoxyethanol	70643-19-5	Hair dye	28
4-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene carbaldehyde	31906-04-4	Fragrance	28
Acrylate copolymer	25133-97-5	Binder	28
Aesculus turbinata seed extract	No CAS	UV-filter	28
Alcohol denat. Sd alcohol 39-b	No CAS	Phthalate	28
Alcohol denat. Sd alcohol 39-c	No CAS	Phthalate	28

Chemical name (common)	CAS number	Main category	Prioritisation Score
Alcohol ethoxylates	No CAS	Non-ionic surfactant	28
Alcohol sulphate C13	No CAS	Anionic surfactant	28
Alkyl phenol ethoxylates	No CAS	Non-ionic surfactant	28
Allantoin paba	4207-42-5	UV-filter	28
Allyl heptanoate	142-19-8	Fragrance	28
Aluminium zirconium tetrachlorohydrex GLY	134910-86-4	Deodorant	28
Ammonium acrylates copolymer	10604-69-0	Waxes	28
Ammonium laureth sulphate	32612-48-9	Anionic surfactant	28
Ammonium lauryl sulphate	2235-54-3	Anionic surfactant	28
Atranol	526-37-4	Fragrance	28
Behentrimonium dimethicone peg-8 phthalate	No CAS	Phthalate	28
Benzophenone-11	1341-54-4	UV-filter	28
Benzophenone-9	76656-36-5	UV-filter	28
Benzopropanal, 4-methyl	5406-12-2	Fragrance	28
Benzotriazolyl dodecyl p-cresol	125304-04-3	UV-filter	28
Benzylidene camphor sulfonic acid	56039-58-8	UV-filter	28
Benzylidenecamphor hydrolyzed collagen sulfonamide	222400-12-6	UV-filter	28
Bis(2-ethylhexyl) phthalate	117-81-7	Phthalate	28
Bis-ethylhexyloxyphenol methoxyphenyl triazine	187393-00-6	UV-filter	28
Bog myrtle	90064-18-9	Insect repellants	28
Bornelone	2226-11-1	UV-filter	28
Butyl Ester of PVM/MA copolymer	25119-68-0	Film forming	28
Butyl methoxydibenzoylmethane	70356-09-1	UV-filter	28
Calcium cerium oxide	No CAS	UV-filter	28
Calcium paraben	69959-44-0	Paraben	28
Calophyllum inophyllum seed oil	241148-25-4	UV-filter	28
Carotenoids	36-88-4	UV-filter	28
Carthamus Tinctorus (safflower) oil	No CAS	Plant extract	28
Ceria/silica	243133-71-3	UV-filter	28
Ceria/silica talc	243133-70-2	UV-filter	28
Cetrimonium dimethicone PEG-7 phthalate	No CAS	Phthalate	28
Cetyl triethylmonium dimethicone PEG-8 phthalate	229327-93-9	Phthalate	28
Chloroatranol	57074-21-2	Fragrance	28
Citrate	126-44-3	Buffering agent	28
Cobalt DNA	No CAS	UV-filter	28
Cocamide FDA	61789-19-3	Surfactant	28
Cocos nucifera (coconut) oil	8001-31-8	Emollient	28
Cumene sulfonate, ammonium salt	37475-88-0	Hydrotrope	28
Cyclodextrin	12619-70-4	Chelating	28
Deschampsia antarctica leaf extract	No CAS	UV-filter	28
Diacetylcurcumin	19697-86-0	UV-filter	28
Diethylhexyl 2,6-naphthalate	127474-91-3	UV-filter	28
Diethylhexyl butamido triazone	154702-15-5	UV-filter	28
Digalloyl trioleate	17048-39-4 , 27436-80-2	UV-filter	28
Diglycol/isophthalates/sip copolymer	240818-59-1	Phthalate	28
Dihydrogenated tallow phthalate	99035-59-3	Phthalate	28
Diisopropyl ethyl cinnamate	No CAS	UV-filter	28
Diisopropyl methyl cinnamate	32580-71-5	UV-filter	28
Dimethicone peg-7 phthalate	No CAS	Phthalate	28
Dimethicone peg-8 phthalate	No CAS	Phthalate	28

Chemical name (common)	CAS number	Main category	Prioritisation Score
Di-methoxycinnamidopropyl ethyldimonium chloride ether	No CAS	UV-filter	28
Dimethyl 2,6-naphthalate	840-65-3	Phthalate	28
Dimethyl paba ethyl cetearyldimonium tosylate	No CAS	UV-filter	28
Dimorpholinopyridazinone	No CAS	UV-filter	28
Diphenyl carbomethoxy acetoxy naphthopyran	169682-22-8	UV-filter	28
Diphenylmethyl piperazinylbenzimidazole	65215-54-5	UV-filter	28
Disodium phenyl dibenzimidazole tetrasulfonate	180898-37-7	UV-filter	28
Di-t-butyl hydroxybenzylidene camphor	123013-10-5	UV-filter	28
Drometrizole trisiloxane	155633-54-8	UV-filter	28
Ethyl dihydroxypropyl paba	58882-17-0	UV-filter	28
Ethyl diisopropylcinnamate	32580-72-6	UV-filter	28
Ethyl methoxycinnamate	99880-64-5	UV-filter	28
Ethyl trimethylbenzoyl phenylphosphinate	No CAS	UV-filter	28
Ethylene/sodium sulfoisophthalate/terephthalate copolymer	No CAS	Phthalate	28
Ethylhexyl bis-isopentylbenzoxazolylphenyl melamine	288254-16-0	UV-filter	28
Ethylhexyl dimethoxybenzylidene dioxoimidazolidine propionate	No CAS	UV-filter	28
Ethylhexyl ferulate	No CAS	UV-filter	28
Ethylhexyl methoxycrylene	947753-66-4	UV-filter	28
Ethylhexyl methoxydibenzoylmethane	No CAS	UV-filter	28
Etocrylene	5232-99-5	UV-filter	28
Fluorescent brightener 367	5089-22-5	UV-filter	28
Globalide	34902-57-3	Musks	28
Glyceryl ethylhexanoate dimethoxycinnamate	No CAS	UV-filter	28
Glyceryl stearate	123-94-4	Waxes	28
Gossypium herbaceum seedcake extract	223749-08-4	UV-filter	28
Hexamidine paraben	93841-83-9	Paraben	28
Hexanediol disalicylate	No CAS	UV-filter	28
Hexyloxy trimethylphenol	148081-72-5	UV-filter	28
Hibiscolide	6706-60-4	Musks	28
Honey	8028-66-8	Emollient	28
Hydrogentated palm oil	68514-74-9	Emollient	28
Hydrolysed corn starch	8029-43-4	Humectant	28
Hydrolysed rice protein	94350-05-7	Conditioning agent	28
Hydrolyzed euglena gracilis extract	No CAS	UV-filter	28
Hydrolyzed olive fruit	No CAS	UV-filter	28
Hydrolyzed wheat bran	No CAS	UV-filter	28
Hydroxyethylcellulose	9004-62-1	Viscosity control	28
Hydroxypropyl methylcellulose phthalate	9050-31-1	Phthalate	28
Hydroxypropyl phenylhydrazinoyl t-butylcarbamate	No CAS	UV-filter	28
Isobutyl acetate	110-19-0	Solvent	28
Isobutyl phenylhydrazinoyl methanesulfonamide	No CAS	UV-filter	28
Isopropyl dibenzoylmethane	63250-25-9	UV-filter	28
Isopropyl methoxycinnamate	5466-76-2	UV-filter	28
Lanolin oil	70321-63-0	Emollient	28
Limonia acidissima bark extract	No CAS	UV-filter	28

Chemical name (common)	CAS number	Main category	Prioritisation Score
Limonia acidissima bark powder	No CAS	UV-filter	28
Magnesium aluminium silicate	1327-43-1, 12511-31-8	Emulsifier	28
m-Aminophenol (Hydrochloride)	51-81-0	Hair dye	28
m-Aminophenol (Sodium salt)	38171-54-9	Hair dye	28
Manganese oxide	11129-60-5	UV-filter	28
Methoxycinnamidopropyl c18-22 alkyldimonium tosylate	No CAS	UV-filter	28
Methoxycinnamidopropyl hydroxysultaine	No CAS	UV-filter	28
Methoxycinnamidopropyl laurdimonium tosylate	No CAS	UV-filter	28
Methoxycinnamidopropyl polysilsesquioxane	No CAS	UV-filter	28
Methoxycinnamoylpropyl silsesquioxane silicate	No CAS	UV-filter	28
Methyl acrylate/methylene drometrizole methacrylate copolymer	No CAS	UV-filter	28
Methylene bis-benzotriazolyl tetramethylbutylphenol	103597-45-1	UV-filter	28
Momordica cochinchinensis seed aril oil	No CAS	UV-filter	28
Musk 89	1922-67-4	Musks	28
Musk amberol	37609-25-9	Musks	28
Musk ambrette	83-66-9	Musks	28
Musk cyclopentenyl propionate	84012-64-6	Musks	28
Musk pentane	35720-57-1	Musks	28
Muskrat musk	No CAS	Musks	28
Neem oil	90063-92-6	Insect repellants	28
Nonoxynol-4	7311-27-5	Waxes	28
Oxobenzoxazinyl naphthalene sulfoanilide	10128-55-9	UV-filter	28
Ozokerite	12198-93-5	Waxes	28
Palmitoyl coffee bean extract	No CAS	UV-filter	28
PEG/PPG-100/70 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-2/5 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-30/10 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-5/10 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-5/20 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-5/30 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-50/20 tocopheryl ether	No CAS	UV-filter	28
PEG/PPG-70/30 tocopheryl ether	No CAS	UV-filter	28
PEG-150 distearate	9005-08-7	Surfactant	28
PEG-25 PABA	116242-27-4	UV-filter	28
PEG-4 Dilaurate	9005-02-1	Emulsifier	28
Phenoxyethylparaben	55468-88-7	Paraben	28
Poloxamer 407	9003-11-7	Non-ionic surfactant	28
Polyacrylamidomethyl benzylidene camphor	113783-61-2	UV-filter	28
Polyacrylate-26	No CAS	UV-filter	28
Polyamide-2	No CAS	Phthalate	28
Polybutene	9003-28-5	Viscosity control	28
Polyester-14	No CAS	Phthalate	28
Polyester-15	No CAS	Phthalate	28
Polyester-16	69847-57-0	Phthalate	28
Polyethylene	9002-88-4	Film forming	28
Polyethylene isoterephthalate	9003-68-3	Phthalate	28
Polyethylene naphthalate	No CAS	Phthalate	28
Polyethylene terephthalate	25038-59-9	Phthalate	28
Polyethylene/polyethylene terephthalate laminated powder (jpn)	No CAS	Phthalate	28

Chemical name (common)	CAS number	Main category	Prioritisation Score
Polyethylene/polypentaerythrityl terephthalate laminated powder (JPN)	No CAS	Phthalate	28
Polymethyl methacrylate/polypentaerythrityl terephthalate/stearate/palmitate laminated powder (jpn)	No CAS	Phthalate	28
Polypentaerythrityl terephthalate	No CAS	Phthalate	28
Polypropylene terephthalate	No CAS	Phthalate	28
Polyquaternium-11	53633-54-8	Film forming	28
Polyquaternium-59	No CAS	UV-filter	28
Polyquaternium-7	26590-05-6	Film forming	28
Polysorbate 40	9005-66-7	Surfactant	28
Polysorbate 60	9005-67-8	Surfactant	28
Potassium butylparaben	38566-94-8	Paraben	28
Potassium ethylparaben	36457-19-9	Paraben	28
Potassium methoxycinnamate	86636-96-6	UV-filter	28
Potassium methylparaben	26112-07-2	Paraben	28
Potassium paraben	16782-08-4	Paraben	28
Potassium phenylbenzimidazole sulfonate	No CAS	UV-filter	28
Potassium propylparaben	84930-16-5	Paraben	28
Propane	74-98-6	Propellant	28
PVP	9003-39-8	Film forming	28
Red petrolatum	28009-03-8	UV-filter	28
Rhyolite powder	No CAS	UV-filter	28
Romandolide	236391-76-7	Musks	28
Rosa moschata oil/extract	No CAS	Musks	28
Ruta graveolens L.	8014-29-7	Fragrance	28
Rutinyl succinate	267006-02-0	UV-filter	28
Sclareol	515-03-7	Fragrance	28
Silicate	12627-13-3	Opacifying	28
Siloxane D6 (decamethylcyclopentasiloxane)	540-97-6	Siloxanes	28
Sodium acetyl cysteinate	19542-74-6	UV-filter	28
Sodium calcium zinc phosphate	No CAS	UV-filter	28
Sodium isobutylparaben	84930-15-4	Paraben	28
Sodium isoferulate	110993-57-2	UV-filter	28
Sodium mango seedate	No CAS	Plant extract	28
Sodium mangoseedate	No CAS	UV-filter	28
Sodium phenylbenzimidazole sulfonate	5997-53-5	UV-filter	28
Sodium urocanate	6159-49-5	UV-filter	28
Sodium/aluminum/iron/sulphate/citrate/hydroxide	No CAS	UV-filter	28
Sodium/aluminum/iron/sulphate/tartarate/hydroxide	No CAS	UV-filter	28
Sorbitan sesquiisostearate	71812-38-9	Emulsifier	28
Soy protein phthalate	No CAS	Phthalate	28
Spirulina platensis powder	223751-80-2	UV-filter	28
Stannous fluoride	77783-47-3	Oral care	28
Stearalkonium dimethicone peg-8 phthalate	No CAS	Phthalate	28
Styrene/acrylates copolymer	25987-66-0	Waxes	28
Sucrose benzoate/sucrose acetate isobutyrate/butyl benzyl phthalate copolymer	No CAS	Phthalate	28
Sucrose benzoate/sucrose acetate isobutyrate/butyl benzyl phthalate/methyl methacrylate copolymer	No CAS	Phthalate	28
Sunflower seed oil ethyl ferulate esters	No CAS	UV-filter	28
Synthetic beeswax	71243-51-1	Emulsifier	28

Chemical name (common)	CAS number	Main category	Prioritisation Score
Synthetic ruby powder	No CAS	UV-filter	28
TEA-lauryl sulphate	139-96-8	Anionic surfactant	28
TEA-phenylbenzimidazole sulfonate	73705-00-7	UV-filter	28
Tert-butyl acetate	540-88-5	Emollient	28
Tetrahydrocurcumin diacetate	52199-86-7	UV-filter	28
Titanium dioxide	13463-67-7	UV-filter	28
Titanium zeolite	No CAS	UV-filter	28
Tocopheryl acetate	52225-20-4	Conditioning agent	28
Tocotrienols	6829-55-6	UV-filter	28
Tonalide	406-02-1	Musks	28
Tosylamide/formaldehyde resin	25035-71-6	Film forming	28
Triclocarbon	101-20-2	Antimicrobial	28
Tripaba panthenol	No CAS	UV-filter	28
Tris-biphenyl triazine	31274-51-8	UV-filter	28
Undecylenoyl peg-5 paraben	No CAS	Paraben	28
VA/Crotonates copolymer	25609-89-6	Film forming	28
Va/crotonates/methacryloxybenzophenone-1 copolymer	No CAS	UV-filter	28
Velvione	37609-25-9	Musks	28
Vitis vinifera seed extract	84929-27-1	UV-filter	28
Zinc adenosine triphosphate hydroxide	No CAS	UV-filter	28
Zinc ascorbate hydroxide	No CAS	UV-filter	28
Zinc azelate hydroxide	No CAS	UV-filter	28
Zinc cerium oxide	No CAS	UV-filter	28
Zinc docosahexaenoate hydroxide	No CAS	UV-filter	28
Zinc isomerized linoleate hydroxide	No CAS	UV-filter	28
Zinc linoleate hydroxide	No CAS	UV-filter	28
Zinc linolenate hydroxide	No CAS	UV-filter	28
Zinc oxide	1314-13-2	UV-filter	28
Zinc retinoate hydroxide	No CAS	UV-filter	28
1-(4'-Nitrophenylazo)-2-methyl-4-bis-(β-hydroxyethyl)aminobenzene	3179-89-3	Hair dye	27
1-Acetoxy-2-methylnaphthalene	5697-02-9	Hair dye	27
2-methyl-1-naphthol	7469-77-4	Hair dye	27
4-[(2-nitrophenyl)amino]phenol	54381-08-7	Hair dye	27
Acetyl tributyl citrate	77-90-7	Fragrance	27
Acid Green 25	4403-90-1	Hair dye	27
Alcohol ethoxylates C15	No CAS	Non-ionic surfactant	27
Alcohol ethoxylates C8	No CAS	Non-ionic surfactant	27
Alcohol ethoxysulphate C15	No CAS	Anionic surfactant	27
Alcohol sulphate C12	No CAS	Anionic surfactant	27
Benzophenone-12	1843-05-6	UV-filter	27
Benzophenone-7	85-19-8	UV-filter	27
Butyl phthalyl butyl glycolate	85-70-1	Phthalate	27
Cetearyl alcohol	67762-27-0, 8005-44-5	Emollient	27
Ci solvent red 23	85-86-9	Hair dye	27
Cocamide DEA	68603-42-9	Surfactant	27
Ethyl acetate	141-78-6	Fragrance	27
Ethylene brassylate	105-95-3	Musks	27
Ethylhexyl triazone	88122-99-0	UV-filter	27
Fatty acid salts C14	No CAS	Anionic surfactant	27
Fatty acid salts C16	No CAS	Anionic surfactant	27
Fatty acid salts C18	No CAS	Anionic surfactant	27

Chemical name (common)	CAS number	Main category	Prioritisation Score
ISOEUGENOL	97-54-1	Fragrance	27
Lanolin alcohol	8027-33-6	Conditioning agent	27
Menthol	1490-04-6	Fragrance	27
Mica	12001-26-2	Opacifying	27
MM (Hexamethyldisiloxane)	107-46-0	Siloxanes	27
Musk banone	3100-36-5	Musks	27
Oleyl alcohol	143-28-2	Emollient	27
Petrolatum	8009-03-8	Emollient	27
Polysorbate 80	9005-65-6	Surfactant	27
Siloxane D4 (octamethylcyclotetrasiloxane)	556-67-2	Siloxanes	27
Sodium benzotriazolyl butylphenol sulfonate	92484-48-5	UV-filter	27
Stearalkonium hectorite	12691-60-0, 94891-33-5	Viscosity control	27
Tea tree oil	68647-73-4	Fragrance	27
Terephthalylidene dicamphor sulfonic acid	92761-26-7 , 90457-82-2	UV-filter	27
Toluene sulfonate, potassium salt	16106-44-8, 30526-22-8	Hydrotrope	27
Triticum vulgare (wheat) germ oil	8006-95-9, 68917-73-7	Emollient	27
Vitamin K1	84-80-0, 11104-38-4, 81818-54-4	Skin lightener	27
Xylene sulfonate, calcium salt	28088-63-3	Hydrotrope	27
Xylene sulfonate, potassium salt	30346-73-7	Hydrotrope	27
AHMI (5-acetyl-1,1,2,3,3,6-hexamethylindan)	15323-35-0	Musks	26
Alcohol ethoxylates ceteareth-20 C16-18	68439-49-6	Non-ionic surfactant	26
Alcohol ethoxysulphate C17	No CAS	Anionic surfactant	26
Alcohol sulphate C14	No CAS	Anionic surfactant	26
Ascorbyl palmitate	137-66-6	Antioxidant	26
Benzyl butyl phthalate; (BBP)	85-68-7	Phthalate	26
Bis(butylbenzoate) diaminotriazine aminopropyltrisiloxane	207562-42-3	UV-filter	26
Bishydroxyethyl biscetyl malonamide	149591-38-8	Conditioning agent	26
Ceteth-2	5274-61-3	Non-ionic surfactant	26
Cetyl alcohol	36653-82-4	Emollient	26
Climbazole	38083-17-9	Preservative	26
Di-cyclohexyl phthalate (DCHP)	84-61-7	Phthalate	26
Ethylene Dodecanedioate	54982-83-1	Musks	26
Magnesium carbonate	546-93-0	Bulking agent	26
Musk R1	3391-83-1	Musks	26
Octocrylene	6197-30-4	UV-filter	26
Oxalide	1725-01-5	Musks	26
Phthalates	No CAS	Phthalate	26
Potassium stearate	593-29-3	Emulsifier	26
Alcohol ethoxylates C13	No CAS	Non-ionic surfactant	25
Alcohol ethoxylates C14	No CAS	Non-ionic surfactant	25
Alcohol ethoxysulphate C16	No CAS	Anionic surfactant	25
Cocamide MEA	68140-00-1	Surfactant	25
Cyclomethicone	556-67-2	Humectant	25
Disodium bisethylphenyl triaminotriazine stilbenedisulfonate	24565-13-7	UV-filter	25
Ethylhexyl dimethyl paba	21245-02-3	UV-filter	25
Ethylhexyl salicylate	118-60-5	UV-filter	25

Chemical name (common)	CAS number	Main category	Prioritisation Score
Homosalate	118-56-9	UV-filter	25
Magnesium stearate	557-04-0	Bulking agent	25
Sorbitan stearate	1338-41-6	Emulsifier	25
Stearic acid	57-11-4	Surfactant	25
AHTN (6-Acetyl-1,1,2,4,4,7-hexamethyltetraline)	21145-77-7, 1506-02-1	Musks	24
Alcohol ethoxylates C12	No CAS	Non-ionic surfactant	24
Alcohol sulphate C15	No CAS	Anionic surfactant	24
Cholesterol	57-88-5	Emollient	24
Esterquats (DEEDMAC, diethyloxyester dimethylammonium chloride)	67846-68-8, 97158-31-1,	Cationic surfactants	24
Ethylhexyl methoxycinnamate	5466-77-3	UV-filter	24
Isoamyl p-methoxycinnamate	71617-10-2	UV-filter	24
Lanolin	8006-54-0, 8020-84-6	Emollient	24
Menthyl salicylate	89-46-3	UV-filter	24
Muscone	541-91-3	Musks	24
Musk moskene	116-66-5	Musks	24
Musk tibetene	145-39-1	Musks	24
Oleic acid	112-80-1	Emollient	24
Squalene	111-02-4	Emollient	24
Thibetolide	106-02-5	Musks	24
Tocopherol	59-02-9	Conditioning agent	24
Traseolide	68140-48-7	Musks	24
1,2-Benzenedicarboxylic acid, dipentylester, branched and linear [1]; n-Pentyl-isopentylphthalate [2]; di-n-Pentyl phthalate [3]; Diisopentylphthalate [4]	84777-06-0 [1] , - , 131-18-0 [3] , 605-50-5 [4]	Phthalate	23
ADBI (4-acetyl-6-tert. butyl-1,1-dimethylindan)	13171-00-1	Musks	23
Alcohol ethoxylates C16	No CAS	Non-ionic surfactant	23
Alcohol ethoxylates C18	No CAS	Non-ionic surfactant	23
Alcohol ethoxysulphate C18	No CAS	Anionic surfactant	23
Alcohol sulphate C16	No CAS	Anionic surfactant	23
Alcohol sulphate C18	No CAS	Anionic surfactant	23
Benzoyl peroxide	94-36-0	Bleaching agent	23
Diethylamino hydroxybenzoyl hexyl benzoate	302776-68-7	UV-filter	23
Diethylhexyl terephthalate	6422-86-2	Phthalate	23
Esterquats (HEQ, Hamburg Esterquat)	19467-38-0	Cationic surfactants	23
Esterquats (TEAQ, triethanol amine quat)	91995-81-2, 93334-15-7, 91032-11-0, 94095-35-9, 85408-12-4,	Cationic surfactants	23
Ethyl methacrylate	688-84-6	Film forming	23
Ethylhexyl palmitate	29806-73-3	Emollient	23
Exaltone	502-72-7	Musks	23
Fatty acid salts >C18	No CAS	Anionic surfactant	23
Myristal myristate	3234-85-3	Emollient	23
Stearyl alcohol	112-92-5	Emollient	23
Galaxolide	114109-62-5, 78448-48-3, 1222-05-5	Musks	22
Isopropyl myristate	110-27-0	Emollient	21
Isopropyl palmitate	142-91-6	Emollient	21

Appendix C Removal during wastewater treatment

Table C.1 presents the removal and fate of the prioritised chemicals in waste water treatment works.

Table C.1 Fate and removal in wastewater treatment works

Chemical name (common)	WwTW minimum removal, %	WwTW maximum removal, %	Fate - minimum % to effluent	Fate - maximum % to effluent	Fate - average % to sludge	Fate - average % biodegraded	Fate - average % volatilised	Reference
(1-hydroxyethylidene) diphosphonic acid (HEDP)	80	>90	10	20	80->90	0	-	HERA (September 2004)
1,2,3-Benzotriazole	29	55	45	71	1	28-54	-	Liu *et al*., (2012)
1H-Benzotriazole, 4(or 5)-methyl-	76	86	14	24	0.5	75-85	-	Liu *et al*., (2012)
2-(2-butoxyethoxy)ethanol (DEGBE)	87	90	10	13	-	87	-	EC (2000), Verschueren (1996)
Amino tris(methylene phosphonic acid) (ATMP)	80	93	7	20	80-93	0	-	HERA (2004).
Benzophenones	62	99	1	38	-	62-99	-	Jennings *et al*., (2009), MITI (1992), Rojas *et al*., (2011), Yu and Zhang (2011)
Bis(2-methoxyethyl) phthalate (Dimethoxyethyl) phthalate - DMEP)	>98	-	2	2	>98	0	-	Oliver *et al*.,(2005)
Boric acid	0	25	75	100	0-25	0	-	HERA (March 2005), Ericksson (2001)
Cocamidopropyl betaine	90	100	0	10	-	-	-	Madsen et al., (2000)
Diethylene glycol ethyl ether (DEGEE)	61	98	2	39	-	61-98	-	Verschueren (1996), Monteith (1987)
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	85	97	3	15	85-97	0	-	HERA (September 2004)
Dimethyl phthalate	93	96	4	7	<0.1	>90	-	Roslev *et al*., (2007), Dargnat, *et al*., (2009

Chemical name (common)	WwTW minimum removal, %	WwTW maximum removal, %	Fate - minimum % to effluent	Fate - maximum % to effluent	Fate - average % to sludge	Fate - average % biodegraded	Fate - average % volatilised	Reference
Ethylenediaminetetraacetic acid (EDTA) derivatives (Inc. Tetrasodium EDTA)	0	0	100	100	0	0	0	Sternbeck and Österås (2012), Verschueren (1996), Kari and Giger (1996)
Fluorescent Brightener FWA-1	85	90	10	15	85-90	0	-	Hera (October 2004), Poiger *et al*., (1998)
Linear Alkylbenzene Sulphonate	89	99	11	1	10-20	80-90	-	HERA (2013), Holt *et al*., (1998), Holt *et al*., (2003)
Methyl paraben	78	99	1	22	-	-	-	USEPA (2010), Eriksson *et al*., (2003), Andersen et al., (2007), Andersen and Larsen (2013)
Methyldibromo glutaronitrile	1	-	99	99	1	0	0	EC (2008)
Musk ketone	80	94	6	20	-	-	-	EC (2005a), Simonich *et al*., (2002), Sabaliunas et al., (2001)
Musk xylene	62	96	4	38	-	-	-	EC (2005b), Simonich *et al*., (2002), Sabaliunas et al., (2001)
N,N-Diethyl-m-toluamide (DEET)	0	91	9	100	-	0-91	-	Jennings *et al*., (2009), Rojas *et al*., (2011), EU (2010)
para-Aminophenol	87	92	8	13	-	90	0	Pitter (1976), Lund (1984)

Chemical name (common)	WwTW minimum removal, %	WwTW maximum removal, %	Fate - minimum % to effluent	Fate - maximum % to effluent	Fate - average % to sludge	Fate - average % biodegraded	Fate - average % volatilised	Reference
Pentasodium pentetate (sodium salt of diethylenetriaminepentaacetic acid - DTPA)	0	0	100	100	0	0	0	Sternbeck and Österås (2012)
Propylene glycol	92	99.5	0.5	8	-	>90	-	CES (1988), EPA (2000)
Salicylic acid	97.0	98.5	1.5	3.0	-	-	-	Miège et al., (2009), Gargošová et al., (2013)
Secondary Alkane Sulphonate	97	99.9	0.1	3.0	15.6	84	-	HERA (April 2005), Arthur. D. Little Inc. (1977)
Siloxane (D4-octamethylcyclotetrasiloxane)	90	98	2	10	90-98	-	-	Environment Agency (2009), Kaj et al., (2005)
Siloxane (D5-decamethyl-cyclopentasiloxane)	91	98	2	9	91-98	-	-	Environment Agency (2009), Kaj et al., (2005)
Siloxane (D6-dodeca-methylcyclohexasiloxane)	90	97	3	10	90-97	-	-	Environment Agency (2009), Kaj et al., (2005)
Sodium Isopropylparaben	78	97	3	22	-	-	-	Andersen et al., (2007)
Sodium Methylparaben	78	99	1	22	-	-	-	USEPA (2010), Eriksson et al., (2003), Andersen et al., (2007), Andersen and Larsen (2013)

Chemical name (common)	WwTW minimum removal, %	WwTW maximum removal, %	Fate - minimum % to effluent	Fate - maximum % to effluent	Fate - average % to sludge	Fate - average % biodegraded	Fate - average % volatilised	Reference
Sulphamic acid	0	0	100	100	-	-	-	ECHA (2013).
Triclosan	79	93	7	21	47%	>30	-	Miège et al., (2009), Thompson et al., (2005), Federle et al., (2002)
Triethanolamine	88	94	6	12	0	0	0	Verschueren (1996), U.S. Environmental Fate and Exposure Potential link at the National Centre for Biotechnology Information

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Appendix D Removal during drinking water

Percentage removal has been based on information found in the referenced sources or, in the absence of data, based on properties (solubility, Log Kow), molecular weight or chemical structure.

C = Coagulation, chemical coagulation based treatment

AC = GAC, Granular Activated Carbon

C, AC = Coagulation and GAC

C, Oz, AC = Coagulation, GAC and ozone

C,Oz, AC, Memb = Coagulation, GAC, ozone and membrane filtration (ultrafiltration (UF) or microfiltration (MF)).

Note: assumption is that chlorination will have little effect on these chemicals.

Chemical	Published removal information	Source	Comments	%Removal
Benzophenone	No data		Log Kow suggest good removal by activated carbon. Chemical structure (benzene ring) suggests some removal by ozone. MW suggests little removal by MF or UF, or by coagulation.	C:0 C,AC:50 C, Oz, AC:70 Memb:0
Siloxane	No data		Log Kow suggest good removal by activated carbon. Chemical structure (no double bonds) suggests poor removal by ozone. MW suggests little removal by MF or UF, or by coagulation.	C:0 C,AC:50 C, Oz, AC:50 Memb:0
1,2,3,- Benzotriazole	No significant removal by chemical coagulation. Poor removal by PAC. Good removal by ozone.	Reemtsma *et al*. (2010)., Karpel Vel Leitner and Roshani (2010)., Wiess *et al*. (2006).	Log Kow and solubility suggest poor-moderate removal by activated carbon. No significant removal by UF or MF expected from MW.	C:0 C,AC:10 C, Oz, AC:90 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Boric acid	No data		No significant removal by chemical coagulation likely. Inorganic, so no removal by activated carbon. Not likely to be oxidized by ozone. No significant removal by UF or MF expected from MW.	C:0 C,AC:0 C, Oz, AC:0 Memb:0
1H- Benzotriazole	No significant removal by chemical coagulation. Poor removal by PAC. Good removal by ozone.	Reemtsma *et al*. (2010)., Karpel Vel Leitner and Roshani (2010)., Wiess *et al*. (2006).	Log Kow and solubility suggest poor-moderate removal by activated carbon. No significant removal by UF or MF expected from low MW.	C:0 C,AC:10 C, Oz, AC:90 Memb: 0
Pentasodium pentetate	No data		Negative Log Kow and high solubility suggest no removal by activated carbon. Unlikely to be removed by chemical coagulation or membranes. C-O double bond structure suggests some removal by ozone.	C:0 C,AC:0 C, Oz, AC:30 Memb: 0
EDTA derivatives	Some removal by ozonation and MF. No removal by coagulation. Up to 80% removal by activated carbon and ozone.	Brauch and Schullerer (1987)., Hrubec *et al.* (1991)., Gilbert and Beyerle (1992)., Drewes *et al*. (2003).	Unlikely to be removed by activated carbon because of negative log Kow.	C:0 C,AC:0 C, Oz, AC:80 Memb: 50

Chemical	Published removal information	Source	Comments	%Removal
1-(hydroxyethylidene) diphosphonic acid (HEDP)	No data		Negative Log Kow and high solubility suggest no removal by activated carbon. Unlikely to be removed by chemical coagulation or membranes. Chemical structure suggests little or no removal by ozone.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Amino tris(methylene phosphonic acid) (ATMP)	No data		Negative Log Kow and high solubility suggest no removal by activated carbon. Unlikely to be removed by chemical coagulation or membranes. Chemical structure suggests little or no removal by ozone.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	No data		Negative Log Kow and high solubility suggest no removal by activated carbon. Unlikely to be removed by chemical coagulation or membranes. Chemical structure suggests little or no removal by ozone.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Secondary alkyl sulphonate	No data		Log Kow suggests some removal by activated carbon, although very high solubility. Unlikely to be removed by chemical coagulation or membranes. Chemical structure suggests little or no removal by ozone.	C: 0 C,AC:20 C, Oz, AC:20 Memb: 0
Sulphamic acid	No data		No significant removal would be expected by coagulation, activated carbon, ozone or MF/UF.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Methyldibromo glutaronitrile	No data		Log Kow and solubility suggest poor to moderate removal by activated carbon. No removal expected from ozone based on chemical structure. Little removal would be expected by coagulation because of high solubility. Low MW suggests no removal by UF or MF.	C: 0 C,AC:10 C, Oz, AC:10 Memb: 0
2-(2-butoxyethoxy)ethanol (DEGBE)	No data		Little removal would be expected by coagulation because of high solubility. High solubility and low log Kow suggest no effective removal by activated carbon. Low MW suggests no removal by UF or MF.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Triethanolamine	No data		High solubility would suggest little removal by coagulation, and with negative log Kow, little removal by activated carbon. Low MW suggests no removal by membranes.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Cocamidopropyl Betaine	No data		High solubility would suggest little removal by coagulation or activated carbon. Low MW suggests no removal by membranes.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Fluorescent brightener FWA-1	No data		Solubility and Log Kow suggest no removal by activated carbon. MW suggests some removal by UF. Unlikely to be any removal by coagulation. Chemical structure suggests some removal by ozone.	C: 0 C,AC: 0 C, Oz, AC: 50 Memb: 10
Dimethyl phthalate	No data for dimethyl phthalate. Other phthalates partly removed by activated carbon, ozone, UF and chemical coagulation.	Whitaker and Moore (1983). Mohan *et al.* (2007)., Lau *et al.* (2005)., Xu *et al.* (2007)., Oh *et al.* (2006)., Bodzek *et al.* (2004)., Medellin-Castillo *et al.* (2013).	Log Kow suggests some removal by activated carbon. Assume removals similar to other phthalates.	C: 30 C,AC: 50 C, Oz, AC: 80 Memb: 50
Linear alkylbenzene sulphonate	No removal by chemical coagulation. Limited removal by activated carbon. Some breakdown by ozone.	Delanghe *et al.* (1991)., Scouten *et al.* (2009)., Tabrizi and Mehrvar (2006.	Log Kow suggests effective removal by activated carbon. MW would suggest little removal by UF or MF.	C: 0 C,AC: 30 C, Oz, AC: 50 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Ethoxydiglycol	No data		Negative Log Kow and high solubility suggest no removal by activated carbon. Low MW so no removal by membranes. Chemical structure suggests no removal by ozone. Removal by coagulation unlikely.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0
Para-aminophenol	No data		Solubility and Log Kow suggest no removal by activated carbon, although some removal of phenol would be expected. Low MW so no removal by membranes. Chemical structure suggests some removal by ozone. Removal by coagulation unlikely.	C: 0 C,AC: 20 C, Oz, AC: 50 Memb: 0
Propylene glycol	No data		Negative log Kow and high miscibility with water suggest no removal by activated carbon. Unlikely to be removed by coagulation. Low MW suggests no removal by UF or NF. Unlikely to be removed by ozone based on chemical structure.	C: 0 C,AC: 0 C, Oz, AC: 0 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Salicylic acid	No effective removal by coagulation. Some removal by activated carbon and ozone. Removal by NF but no data for UF or MF.	Tseng *et al*. (1989)., Semmens and Ayers (1985). Cathalifaud *et al*. (1995)., Matthews (1990)., Rahni and Legube (1996). De Laat *et al*. (1984)., De Laat *et al*. (1985). Tseng *et al*. (1990)., Scheck and Frimmel (1995). Duguet *et al*. (1987)., Eall and Vanloon (2000)., Karpel Vel Leitner *et al*. (1999).	Log Kow suggests removal by activated carbon. Low MW suggests no removal by UF or MF. Chemical structure suggests some removal by ozone.	C: 0 C,AC: 30 C, Oz, AC: 60 Memb: 0
Bis(2-methoxy) phthalate	No data		Log Kow suggests moderate removal by activated carbon. No removal likely by coagulation or membranes. Chemical structure suggests some removal by ozone.	C: 0 C,AC: 30 C, Oz, AC: 40 Memb: 0
Methyl paraben	Suggestions that ozone could be effective.	Verschueren (1996).	Log Kow suggests some removal by activated carbon. Unlikely to be removed by coagulation or membranes (low MW).	C: 0 C,AC: 40 C, Oz, AC: 60 Memb: 0
Sodium isopropylparaben	No data		Log Kow and solubility suggest some removal by activated carbon. Unlikely to be removed by coagulation or membranes (low MW). Chemical structure suggests some removal by ozone.	C: 0 C,AC: 20 C, Oz, AC: 40 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Sodium methylparaben	No data		Log Kow and solubility suggest some removal by activated carbon. Unlikely to be removed by coagulation or membranes (low MW). Chemical structure suggests some removal by ozone.	C: 0 C,AC: 20 C, Oz, AC: 40 Memb: 0
DEET	No data		Log Kow and solubility suggest some removal by activated carbon. Unlikely to be removed by coagulation or membranes (low MW). Some removal likely by ozone based on chemical structure.	C: 0 C,AC: 20 C, Oz, AC: 40 Memb: 0
Triclosan	No data		Log Kow and solubility suggest good removal by activated carbon. Unlikely to be removed by coagulation or membranes. Some removal likely by ozone based on chemical structure.	C: 0 C,AC: 50 C, Oz, AC: 70 Memb: 0

Chemical	Published removal information	Source	Comments	%Removal
Musk ketone (nitro-musks)	Some removal by coagulation and activated carbon. Some reduction by UF, but not ozone.	Neamtu *et al.* (2000)., Westerhoff *et al.*(2005)., Snyder *et al.* (2007)., Yoon *et al.* (2006)., Janzen *et al.* (2011).		C: 20 C,AC: 50 C, Oz, AC: 50 Memb: 20
Musk xylene nitro-musk	Some removal by coagulation and activated carbon. Some reduction by UF, but not ozone.	Neamtu *et al.* (2000)., Westerhoff *et al.*(2005)., Snyder *et al.* (2007)., Yoon *et al.* (2006)., Janzen *et al.* (2011).		C: 20 C,AC: 50 C, Oz, AC: 50 Memb: 20

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Appendix E Exposure estimates through typical use

WRc Ref: DWI9879.03/15903-0
June 2014

Table E.1 Estimated exposure through typical use of the PCPs and DCPs

Chemical name (common)	SED mg/kg bw/day	Derivation	Reference
(1-hydroxyethylidene) diphosphonic acid (HEDP)	0.00053	Exposure via direct or indirect skin contact, inhalation and oral routes.	HERA (2004b).
1,2,3-Benzotriazole	1.67E-05	Based on extrapolation from measured urinary concentrations of 6 benzotriazoles (1H-benzotriazole, 1-hydroxy-benzotriazole, 4- and 5-hydroxybenzotriazole [mixture of two isomers], tolyltriazole, xylyltriazole [or 5,6-dimethyl-1H-benzotriazole], and 5-chloro-benzotriazole)) in the US.	Asimakopoulos *et al* (2013)
1H-Benzotriazole, 4(or 5)-methyl-	1.67E-05		
2-(2-butoxyethoxy)ethanol (DEGBE)	0.00043	Total human daily intake via air, drinking water, and food resulting from use in detergent products.	HERA (2005a).
Amino tris(methylene phosphonic acid) (ATMP)	0.00053	Exposure via direct or indirect skin contact, inhalation and oral routes.	HERA (2004b).
Benzophenones	1.89	Based on exposure to BP-3 as a UV-filter in sunscreens and cosmetic formulations. No exposure estimates located for other benzophenones.	SCCP (2008a).
Bis(2-methoxyethyl) phthalate	0.00913	Based on dermal exposure to dibutyl phthalate, since DBP is reported to have raised the most concern in the phthalate safety assessment. Dimethyl phthalate has a slightly different spectrum of product usage, but the concentrations in those products are fairly similar.	CIR (2005).
Boric acid	0.0000421	Exposure due to hand laundry washing, laundry pretreatment with neat product and misuse of product for hand dishwashing. Indirect exposure via skin contact, exposure via inhalation and exposure via the oral route are all expected to be negligible.	HERA (2005b).
Cocamidopropyl betaine	0.0107	Exposure via direct or indirect skin contact, inhalation and oral routes.	HERA (2005c).

Chemical name (common)	SED mg/kg bw/day	Derivation	Reference
Diethylene glycol ethyl ether (DEGEE)	1.97	Dermal exposure from all cosmetic products, except for oral hygiene and eye products, at a concentration up to 1.5%.	SCCP (2008b).
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	0.00053	Exposure via direct or indirect skin contact, inhalation and oral routes.	HERA (2004b).
Dimethyl phthalate	0.00913 (phthalates)	See Bis(2-methoxyethyl) phthalate	CIR (2005).
EDTA derivitives (Inc. Tetrasodium EDTA)	0.00001 (Tetrasodium EDTA)	Dermal exposure of consumers.	EU RAR (2004).
Fluorescent Brightener FWA-1	0.23	Exposure via direct or indirect skin contact, inhalation of detergent dust or via the oral route.	HERA (2004a).
Linear Alkylbenzene Sulphonate	0.04	Dermal exposure from DCPs and PCPS.	OECD SIDS (2005).
Methyl paraben	0.59	Estimated systemic dose for an adult (single paraben).	CIR (2008).
Methyldibromo glutaronitrile	-	No exposure estimate located: Use of MDGN in cosmetic products banned in the EU, primarily due to sensitisation. No estimate of exposure due to continued use in DCPs located.	SCCP (2006).
Musk ketone	0.20029	Total dermal exposure from various cosmetics and from detergents.	EU RAR (2005a).
Musk xylene	0.2066	Total dermal exposure from various cosmetics and from detergents.	EU RAR (2005b).
N,N-Diethyl-m-toluamide (DEET)	1.02	Based on average Absorbed Daily Dosage (ADD) for an adult male weighting 78 kg.	California EPA (2000)
para-Aminophenol (PAP)	Negligible	PAP is metabolised to APAP in the skin, and so topical application of PAP is reported to result in systemic exposure to APAP but not to PAP. Likely that the situation is similar after oral exposure.	SCCP (2005).
Pentasodium pentetate	-	No exposure estimate located.	-

Chemical name (common)	SED mg/kg bw/day	Derivation	Reference
Propylene glycol	0.72	Used as a food additive. Average daily dietary intake in Japan in 1982 estimated to be 43 mg per person per day (0.72 mg/kg bw/day based on a 60 kg adult). Note that this is old data. Considered to be Generally Recognised As Safe (GRAS). Acceptable Daily Intake (ADI) is 25 mg/kg bw/day; this was set by JECFA in 1974 and is still current.	JECFA (1974).
Salicylic acid	0.5	Representative exposure to one cosmetic product (dermal exposure); simultaneous use of multiple cosmetic products containing salicylic acid considered unlikely. For comparison, exposure from ingestion of a low-dose regimen (81 mg) aspirin by a 58 kg female is approximately 1.4 mg/kg bw/day.	CIR (2003).
Secondary Alkane Sulphonate	0.00387	Exposure via direct or indirect skin contact, inhalation or oral routes. Included in this estimate is exposure from dishwashing, laundry and cleaning products. Not included - exposure from cosmetics hair, body care products and industrial cleaners.	HERA (2005d).
Siloxane (D4-octamethylcyclotetrasiloxane)	0.243	Total exposure from PCPs.	Health Canada (2008c).
Siloxane (D5-decamethyl-cyclopentasiloxane)	0.16	Total exposure from PCPs.	Health Canada (2008b).
Siloxane (D6-dodeca-methylcyclohexasiloxane)	0.085	Total exposure (via inhalation, dermal and oral routes) from PCPs for an adult female.	Health Canada (2008a).
Sodium isopropylparaben	0.59	Estimated systemic dose for an adult (single paraben).	CIR (2008).
Sodium methylparaben	0.59	Estimated systemic dose for an adult (single paraben).	CIR (2008).
Sulphamic acid	-	No exposure estimate located.	-
Triclosan	0.5661	Total exposure to oral products and dermal formulations (leave-on and rinse-off products).	SCCP (2009). Triclosan
Triethanolamine	11.44	Dermal exposure of consumers, assuming 2.5% TEA in cosmetic products.	CIR (2011).

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