Comprehensive mass flow analysis of Swedish sludge contaminants

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\textbf{Abstract}

A screening of metals, persistent organic pollutants, pharmaceuticals and personal care products (PPCPs), and other organic contaminants in sludge from seven Swedish sewage treatment plants (STPs) was performed in this study. This extensive screening provides information on mass flows of 282 compounds used in the Swedish society to sewage sludge. It reveals constant relative contaminant concentrations (ng-mg kg\textsuperscript{-1} d.w.), except for some pesticides and perfluorinated compounds, indicating that these originate from broad usage and diffuse dispersion rather than (industrial) point sources. There was a five order of magnitude difference in the sum concentrations of the most and least abundant species (metals and polychlorinated dibenzo-\textit{p}-dioxins and -furans, respectively). Lower total concentrations were found in sludge from STPs processing primarily food industry or household sewage. Proportions of the amounts used (in Sweden) found in sludge were lower for compounds that are present in consumer goods or are diffusely dispersed into the environment (0.01-1\% recovered in sludge) than for compounds used as detergents or PPCPs (17-63\%). In some cases, the recovery seemed to be affected by evaporation (e.g. octamethylcyclotetrasiloxane) or biotransformation (e.g. adipates) losses, while polychlorinated alkanes and brominated diphenyl ethers were recovered to disproportionately high degree (ca.4\%); likely due to incomplete statistics for imported goods.

\textit{Keywords:} PPCP, POP, sewage sludge, emerging pollutants.

\textbf{Highlights:}

- We have performed an extensive screening of sewage sludge contaminants.
- Overall levels and distribution patterns of the contaminants were quite similar between the sewage treatment plants (STPs).
- Levels of sludge contaminants seem to be independent on location, size and treatment technique of the plants.
- Types of human activities connected to STPs, generally, did not affect the levels of sludge contaminants.
1. Introduction

Municipal sewage treatment plants (STPs) process sewage from a variety of sources, e.g. households, industrial sites, and hospitals, and the final solid product is usually dewatered digested sludge. Sludge contains nutrients and organic matter that should be used in agriculture as soil improvement, but also substances that pose environmental and health hazards. The fate of chemicals during sewage treatment depends on both the treatment process and the nature of the substance; by volatilization, biodegradation, sorption to sludge or discharging into recipient water (Zitomer and Speece, 1993). STPs can be considered as secondary sources of pollutants discharged into the environment (Harrison et al., 2006; Kinney et al., 2006; Xia et al., 2005).

Large quantities of pharmaceuticals and personal care products (PPCPs) may enter the aquatic environment via STPs and due to their negative effects on aquatic organisms (DeLorenzo and Fleming, 2008; Kuriyama et al., 2005; Muirhead et al., 2006) PPCPs are classified as emerging pollutants. Domingo and Bocio (2007) concluded that frequently high consumption of certain fish species could increase the health risks by polychlorinated dibenzo-p-dioxins and -furans (PCDD/Fs) and polychlorinated biphenyls (PCBs) intake. Results from intake studies (Darnerud et al., 2006; Kiviranta et al., 2004; Schecter et al., 2001) concluded that levels of persistent organic pollutants (POPs) in fish are generally higher compared to other foods. Darnerud et al. (2006) also showed that fish (major), meat, dairy products, and fats/oils are sources to POPs intake for Swedish consumers. Harrison et al. (2006) concluded that more data are needed on contaminant concentrations in sludge as well as temporal trends to enhance our knowledge about their presence in sludge. This is especially of importance during risk assessment of land applications of sludge and to identify needs (if any) for further restrictions. As phosphorus resources will be depleted (Steen, 1998), land applications of biosolids (treated sewage sludge) are important in terms of sustainable nutrient management. Clarke and Smith (2011) concluded that emerging organic compounds (OCs) will not put human health at risk when recycling biosolids on land.

In Sweden, the annual production of STP sludge amounts to approximately 240000 tonnes dry weight (d.w.) per year (Swedish EPA, 2007), with phosphorus and nitrogen contents of ca. 3% and 3.5%, respectively. Optimizing the use of these nutrients in the sludge could be highly significant in terms of conserving resources. According to a Swedish Government decision, by 2015 at least 60% of the phosphorus originating from sewage should be returned to productive soil, half of which should be applied to arable land (Swedish EPA, 2002; Wallgren, 2001). The strategy for meeting this objective includes: (i) increasing the recovery of nutrients and (ii) reducing the contents of hazardous substances. The greatest challenge may be to reduce the contents of hazardous substances in sludge and sludge-amended soil sufficiently to fulfill legal requirements and to convince consumers and consumer organizations that products grown on such amended soil are safe.

The purposes of this study were to: (i) perform a screening of metals, POPs, PPCPs, and other OCs in sludge from Swedish STPs with various characteristics; (ii) investigate possible correlations between the annual quantities used in Sweden and the measured concentrations in sewage sludge; (iii) assess whether the percentages found in sludge (relative to the amounts used) are related to physicochemical properties or biodegradability of the pollutants; (iv) examine distribution patterns between and within STPs; and (v) identify potential sources of considered pollutants (e.g. domestic, industrial or storm water).
2. Material and methods

2.1 Selection of compounds and STPs

The target compounds and the STPs were selected together with the Swedish EPA, additional information can be found in supplementary data. Main application areas for the compounds and annual quantities used in Sweden (2004) are summarized in Table 1, and physicochemical properties in Table 2 and S1. Table 3 and Fig.S1 presents descriptive data of the STPs.

2.2. Analysis and data evaluation

The analyses were performed by several qualified laboratories, each following strict quality guidelines. Generally, internal standard quantification was used to compensate for losses during clean-up and analysis. For non-accredited analyses the extraction efficiencies were checked (e.g. using re-extraction) and found to be sufficient (better than 95%). The uncertainties of the analytical methods were in the range 20-40% (for detailed information on the analytical techniques applied see Table S2).

Mass flows (MFs) of the compounds were calculated, based on the measured concentration (MC) and the annual production (in Sweden) of sewage sludge, assuming that all sludge generated is spread on land (that is a reasonable approximation, since only small proportions are incinerated). To assess the proportions of the substances used in the technosphere that reach the STPs and associate with sludge, MFs were compared to the recorded amounts used in Sweden (Swedish Chemicals Agency, 2007b).

Principal component analysis (PCA), a multivariate data analysis tool, was used (SIMCA-P+11; Umetrics, Sweden) to extract and visualize major patterns and trends in the data and to generate an easily interpreted overview of the results. The PCA model includes the compounds that have been analyzed in all STPs (n=7) and results <LoD (limit-of-detection) were set to ½LoD. The data were mean centered and scaled to unit variance to make all parameters equally important.

3. Results and discussion

3.1. Sludge quality

The total and relative concentrations of the target compounds (Table 4 and S3) were found to be comparatively constant on d.w. basis, indicating that sludge contaminants originate from broad usage and diffuse dispersion rather than from (industrial) point sources, even though industries also contribute to chemical constituents in the sludge. Lower levels of the pollutants (35%, on average) were detected in sludge from STPs C and G, processing large quantities of water from a food industry (rich in organic substances and lean in pollutants) and household sewage (lower in industrial pollutants), respectively, than in sludge from the other STPs.

Currently there is European maximum residue limits (MRLs) established for seven metals (in Sweden: Cd, 2; Cr, 100; Cu, 600; Hg, 2.5; Ni, 50; Pb, 100; and Zn, 800 mg kg\(^{-1}\) d.w.) in sludge for agricultural purposes; there are no legal limits for OCs. However, recommended limit values (Sweden) have been set for three groups of “indicator” OCs, i.e. PAHs (3 mg kg\(^{-1}\) d.w.), PCBs (0.4 mg kg\(^{-1}\) d.w.), and 4-nonylphenol (50 mg kg\(^{-1}\) d.w.) (Swedish EPA et al., 1995). All pollutants measured in
this study were below their respective limit. This also applies to the suggested limits in the EC “Working document on sludge” (CEC, 2000) (Di-(2-ethylhexyl) phthalate, DEHP, 100; 4-nonylphenol, 50; ∑PAH, 6; and ∑PCB, 0.8 mg kg⁻¹ d.w.; PCDD/Fs, 100 ng TEQ kg⁻¹ d.w.).

In order to obtain an overview of the sludge contaminants, currently not regulated, the median of the total concentration of each group of compounds detected at each STP was used (Fig.1). There was a five order of magnitude difference in the total concentrations; with metals detected in highest and PCDD/Fs in lowest concentrations. Currently, the EC is assessing if the more than 20-year old sludge directive should be reviewed and revised (http://ec.europa.eu/environment/waste/sludge/index.htm). The data generated in this and other studies provide a wider database of sludge contaminants and aid in the discussions of future limit values.

3.2. Use pattern and sludge contaminant mass flows

The intended use of consumer chemicals, the principal emission routes from articles in use in society (molecular or particulate) and long-range air transport (reaching the sewer system via storm water systems) will all affect the sludge quality. In the case of emissions from consumer articles it is expected that molecular emissions are (relatively) more important for volatile compounds and particulate emissions more important for semi-volatile (high molecular weight) compounds. Comparisons of quantities used in the Swedish society and annual MFs for sludge (Table 4) may be utilized to identify use related, STP treatment related, and other factors affecting the sludge quality.

Metals are used in large quantities in the society and this is reflected in the MF-value (190 tonnes year⁻¹) which is highest of all compound classes. Of the remaining abundant compound classes (with MFs>250 kg year⁻¹) a majority originates from PPCPs (siloxanes, triclosan (antibacterial), BHT (antioxidant), and fluoroquinolone (FQ) and tetracycline (TC) antibiotics), detergents (4-nonylphenol) or pesticides (incl. biocides); products that are used in such a way that release to the sewer system is inevitable. Many of these compounds (siloxanes, 4-nonylphenol, FQs, TCs, and triclosan) have high affinity to sludge (Buyuksonmez and Sekeroglu, 2005; IVL, 2005; Lindberg et al., 2006; Ying and Kookana, 2007). Consequently, it is logical that high proportions of the used amounts are recovered in sludge. Of the annual quantities used in Sweden, 63% of the FQs, 51% of the TCs, 41% of 4-nonylphenol, 29% of triclosan, and 17% of the siloxanes were found sorbed to sludge.

High MFs (>10 tonnes year⁻¹) were also obtained for two groups of high volume plastic additives (Table 4), phthalates (plasticizers) and polychlorinated alkanes (PCAs; flame retardants and plasticizers). These pollutants are presumably evaporating at a low rate from plastic materials, partitioning to dust, and reach the sewage system following cleaning of indoor environments. Although the emission rate is expected to be low, the stock of plastic materials in society is large and the resulting total emitted amounts substantial.

The percentages of PCAs, and the closely related polybrominated diphenylether flame retardants (PBDEs), found sorbed on sludge were remarkably high (4.1 and 3.7%, respectively) – much higher than for organophosphate triesters (OPs; plasticizers and flame retardants) and phthalates (0.06 and 0.04%, respectively). Since all of these classes of compounds have low volatility and, thus, presumably low emission rates, the 10-fold higher percentages recovered of PCAs and PBDEs are hard to explain by intrinsic physicochemical properties. Instead, it may be due to limitations of the national use statistics, not including chemicals in imported articles. It is likely that considerable
amounts of PCAs and PBDEs are entering the country as (unrecorded) additives in imported textiles, plastic articles, computers, and other electronic goods, etc. Many of the compounds that were found at relatively low concentrations in sludge (average concentration < 1 mg kg\(^{-1}\) d.w.; MFs ≤ 0.15 tonnes), e.g. polycyclic aromatic hydrocarbons (PAHs), organotin compounds (OTCs), terpene, chlorophenols (CPs), PCBs, polychlorobenzenes (PCBz), perfluorochemicals (PFCs) and PCDD/Fs stem from multiple, often diffuse sources, such as traffic and long-range air transport, that can reach STPs via storm water systems. For these chemicals it is difficult to make meaningful comparisons with use statistics.

3.3. Factors affecting mass flows

It should be noted that many other factors, in addition to loads of pollutants at STPs, affect their levels in the sludge. The pollutants may, for instance, evaporate/degrade during the treatment process, or pass the STP due to highly water solubility and low sludge affinity. These processes are often related to the physicochemical characteristics (Table 2 and S1) and biodegradability of the compounds.

3.3.1. Evaporation

The volatility of the contaminants may affect the MF-values in two ways; it may (i) affect the initial emission rates of additives in consumer articles and (ii) affect the evaporative losses in the sewage treatment process. A linear relation was observed between the molecular weights of plastic additives and the percentage recovered in sludge (R\(^2\)=0.94; Fig.2), which may indicate that the latter process is more important than the first (for these compounds). However, the compounds included in Fig.2 have such low vapor pressure (Henry’s law constants < 10\(^{-5}\) atm m\(^3\) mol\(^{-1}\)) that substantial evaporation is unlikely. These compounds are therefore most likely emitted from consumer articles mainly through particulate emissions or leaching upon washing or cleaning (OPs; water solubility’s > 5 mg L\(^{-1}\); Table S1).

Evidence for considerable evaporative losses in STPs was however found for cyclic methylsiloxanes. The proportion of their quantities used that reach STPs and sorb to sludge seems to strongly depend on their vapor pressures, which decrease with the number of siloxane units. Octa- (D4), deca- (D5), and dodeca-methylcyclotetrasiloxane (D6) were recovered at 1.3%, 17%, and 54%, respectively. The losses may occur either during biological sewage treatment or sludge digestion. The latter process is known to result in tainted biogas that cause deposits in boilers fed such fuel (Dewil et al., 2006, 2007). Similarly, volatilization is probably the reason for the relatively low recovery of limonene (0.46%).

3.3.2. Biodegradation

Unlike the other PPCPs, the non-steroid anti-inflammatory substances (NSAIDs) were recovered to a low degree (0.04%) in sludge, which may indicate biodegradation and/or passage through STPs in aqueous phase. The latter explanation is less likely as antibiotics are more water soluble and recovered to a greater extent (about 50%). Moderate (diclofenac; 32%) to high (ibuprofen, naproxene, and ketoprofen; 65-90%) removal efficiencies has been reported for Swedish STPs (IVL, 2006). The cited study also showed that the removal efficiency varies considerably between STPs,
and that the removal efficiency tends to be lower in STPs located in the northern part of Sweden, possibly due to lower water temperatures (and lower biological activity).

The percentage recovered of long-chain phthalates (Fig.2) seems to correlate to their molecular weight, maybe due to less availability for biodegradation of the larger molecules. Similarly, of the eight adipates investigated, only the largest (di-(2-ethylhexyl) adipate, DEHA) was detected in sludge. Earlier studies have reported that most of the phthalates are biodegradable in sludge (Liang, et al. 2008).

Biodegradation may also be responsible for the low percentage (0.01%) of tributyl phosphate (TBP) recovered in sludge (Fig.2). TBP has lower water solubility than tris(2-chloropropyl) phosphate (TCPP) and should therefore associate more strongly to sludge, but are still recovered to a 10-fold lower degree. From reports in the scientific literature it is known that TBP and other aliphatic OPs are more degradable than aromatic OPs (e.g. triphenyl phosphate, TPP) and that chlorinated OPs (e.g. TCPP) are most persistent (Saeger et al., 1979; WHO, 1991a, 1991b, 1998).

3.3.3. Water solubility
The proportions of OPs found in the sludge (0.06%) were much lower than PCAs and PBDEs (Table 4) although they are used in similar applications. This may be partially due to recent substitution of the latter by OPs that will immediately influence the statistics, but only slowly affect the levels in sludge (due to long lifetime and large stocks in use). However, the OPs generally have higher biodegradability (3.3.2.) and higher water solubility than PBDEs. Hence, larger proportions of these substances may be degraded or pass through STPs. Chlorinated OPs such as tris(2-chloroethyl) phosphate (TCEP) and TPP are both persistence and water soluble and have been shown to pass STPs to a great extent (Marklund et al., 2005).

3.4. Detection of point sources and differences in use pattern
The PCA model was generated to obtain an overview of the relationships between individual pollutant concentrations (or groups of pollutants) and individual STPs (or groups of STPs). Points representing all STPs, except STP E, cluster near the origin of the score plot (Fig.3a), indicating that these plants have similar pollutant profiles. STPs A, B, D, and F are separated to some degree from STPs C and G, generating sludge with lower overall pollutant levels than the other STPs, hence confirm earlier statement (3.1.).

The PCA loading plots show that sludge from STP E has higher proportions of most PFCs (Fig.3b and Fig.S2) – various pesticides (Fig.3c), hexachlorobenzene (HCBz), highly chlorinated PCDD/Fs (Fig.3d), 4-nonylphenol (4NP) and PBDE 209 (Fig.3e) than the other STPs. The high levels of PFCs in its sludge may be related to textile factories and associated facilities that are connected to STP E and may use these substances during their manufacturing processes or, alternatively, the compounds may be present in imported materials they use. The relatively high levels of the highly chlorinated PCDD/Fs may be related to use of pentachlorophenol as fungicide, e.g. during storage/transport of fabrics, consistent with previous analyses of various municipal solid waste fractions that have shown that the textile fraction contains highest percentages of total PCDD/Fs (Hedman et al., 2007). It may be worth noting that the Swedish textile industry no longer uses perfluoroalkylsulfonates (PFOS, PFDS, PFHxS), and that the STP handling sewage from the textile industry (STP E) contains similar concentrations of PFOS as the other STPs. In fact, sludge from the two largest STPs (A, B) and STP D
contains more perfluoroalkylsulfonates than STP E. Imported products that contain PFCs (excluded in the product register) are assumed to be the primary current sources of PFCs in Swedish STPs.

Sludge from STPs A, B, and D also contains large proportions of metals, antibacterial agents (triclosan and OTCs), and two phthalates (DEHP and di-iso-nonyl phthalate, DINP) that are used as plasticizers in polyvinyl chloride (PVC). These cities are growing rapidly, as their traffic intensity, which may explain the high metal and phthalate levels. The elevated levels of zinc and lead may stem from brake linings of motor vehicles (Hjortenkrans et al., 2007) and metal plated roofs, and the phthalates from building materials. The detection of DEHP at relatively high levels (mg kg\(^{-1}\) d.w.), although it has mainly been substituted by DINP since early 2000 (Peterssson, 2004; Swedish Chemicals Agency, 2007a), indicates that there may be a considerable time lag between regulatory actions and a corresponding drop in pollutant levels, due to the large amounts of DEHP remaining in the technosphere. In one case, STP D, industrial production of vinyl flooring was identified as a possible contributor. Furthermore, all three cities have relatively young and dynamic populations that are likely to buy/use more sports/functional clothing (often containing PFCs/antibacterial agents) than the populations connected to the other STPs.

Sludge produced by the two STPs (C, G) with lowest sludge contaminant levels has relatively high proportions of the fungicide propiconazole, which is primarily applied to barley crops. These STPs are situated in agricultural areas and STP C processes waste from a major food-processing plant, which may explain the occurrence of propiconazole in its sludge.

4. Conclusion

The overall levels and distribution patterns of the sludge contaminants are quite similar, hence these parameters do not seem to be dependent on either the location/size/treatment technique of the plants, or generally the types of human activities that affect the waste streams they handle. Using PCA, minor variations in pollutant levels and patterns were identified and attributed to potential sources. There were clear differences in the PFC distribution patterns between the STPs that could be related to textile industries around STP E, and the occurrence of relatively high levels of propiconazole in sludge from STPs C and G could be associated with agricultural activities.

The proportions of the amounts used found in sludge were generally lower for compounds that are incorporated in consumer goods than for compounds used as detergents or PPCPs and pollutants emitted from point sources. Some (weak) correlations were found between the national use statistics of the chemicals and their measured concentrations in sludge. However, the product registry does not include chemicals in imported goods. Even for articles produced in Sweden it is difficult to determine how much of the various chemicals actually are emitted from the products and reach the sewage system. Thus, there is a need for generic reliable emission models for chemicals in consumer articles.

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Supplementary data
Additional information regarding the selection of the OCs, sample collection, analysis and QA/QC, location of the STPs, distribution patterns of PFCs, CAS numbers, physicochemical properties, analytical techniques applied, uncertainties in the analyses, and sludge concentrations are presented in supplementary data.

References

Kiviranta, H., Ovaskainen, M. A. L., Vartiainen, T., 2004. Market basket study on dietary intake of PCDD/Fs, PCBs, and PBDEs in Finland. Environ. Int. 30(7), 923-932.


Table 1 Primarily applications and annual quantity (in Sweden) of the compounds

<table>
<thead>
<tr>
<th>Compounds</th>
<th>n(^a)</th>
<th>Applications</th>
<th>Quantity (10(^3) kg year(^{-1}))(^b)</th>
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<tbody>
<tr>
<td>As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn</td>
<td>10</td>
<td>Metals</td>
<td>21 046</td>
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<tr>
<td>Phthalates</td>
<td>8</td>
<td>Softening agent in plastics</td>
<td>73 964</td>
</tr>
<tr>
<td>Biocides</td>
<td>11</td>
<td>Killing living organisms</td>
<td>1 637</td>
</tr>
<tr>
<td>Polycyclic aromatic hydrocarbons (PAHs)</td>
<td>6</td>
<td>Products of incomplete combustion</td>
<td>1 203(^c)</td>
</tr>
<tr>
<td>Adipates</td>
<td>8</td>
<td>Softening agent in plastics</td>
<td>1 073</td>
</tr>
<tr>
<td>Pesticides</td>
<td>109</td>
<td>Control pests</td>
<td>828</td>
</tr>
<tr>
<td>Polychlorinated alkanes (PCAs)</td>
<td>3</td>
<td>Lubricants and cutting fluids (metal working industry), and plasticizers</td>
<td>298</td>
</tr>
<tr>
<td>Organophosphorus compounds (OPs)</td>
<td>6</td>
<td>Flame retardants and/or plasticizers in textiles, plastics, and building materials</td>
<td>286</td>
</tr>
<tr>
<td>Butylhydroxytoluene (BHT)</td>
<td>1</td>
<td>Stabilizer in plastics and rubber, antioxidant (ex. processed food)</td>
<td>254</td>
</tr>
<tr>
<td>Organotin compounds (OTCs)</td>
<td>6</td>
<td>In anti-fouling compositions and stabilizer in polyvinyl chloride (PVC)</td>
<td>240</td>
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<tr>
<td>Non-steroid anti-inflammatory drugs (NSAIDs)</td>
<td>4</td>
<td>Pharmaceuticals</td>
<td>84(^d)</td>
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<tr>
<td>Siloxanes</td>
<td>7</td>
<td>Sanitary articles, lubricants and hydraulic fluids in textiles and skin care products</td>
<td>31</td>
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<td>Perfluorochemicals (PFCs)</td>
<td>13</td>
<td>Water, fat or stain repellents for paper, textiles, carpets, etc.</td>
<td>24(^e)</td>
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<td>Terpene (Limonene)</td>
<td>2</td>
<td>Flavor and odor additive (hygiene products and perfumes)</td>
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<tr>
<td>Polychlorobenzenes (PCBz)</td>
<td>11</td>
<td>Dyestuffs and solvent for pesticides</td>
<td>8.1(^f)</td>
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<td>4-Nonylphenol</td>
<td>1</td>
<td>Detergent, surfactants (metabolite)</td>
<td>7.6</td>
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<td>Fluoroquinolones (FQs)</td>
<td>3</td>
<td>Pharmaceuticals (antibiotics)</td>
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<td>Polybrominated diphenylethers (PBDEs)</td>
<td>8</td>
<td>Flame retardants in electronics, furniture, and building materials</td>
<td>3.6(^h)</td>
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<td>Triclosan</td>
<td>1</td>
<td>Antibacterial in toothpaste and deodorants (personal care products)</td>
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<td>Pharmaceuticals (antibiotics)</td>
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<td>4</td>
<td>Pharmaceuticals</td>
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<td>Chlorophenols (CPs)</td>
<td>19</td>
<td>Wood and textile preservatives</td>
<td>Banned (1978)(^j)</td>
</tr>
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<td>Polychlorinated biphenyls (PCBs)</td>
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<tr>
<td>WHO-PCBs</td>
<td>12</td>
<td>Dielectric fluids in transformers and capacitors</td>
<td>Banned (1972)(^j)</td>
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<tr>
<td>Indicator-PCBs (I-PCBs)</td>
<td>7</td>
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<td></td>
</tr>
<tr>
<td>Polychlorinated dibenzo-p-dioxins and furans (PCDD/Fs)</td>
<td>17</td>
<td>Unintentionally formed (by-products)</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^a\) n: number of compounds included in the group. \(^b\) Annual quantity, in Sweden 2004, recorded in the products and pesticides register (Swedish Chemicals Agency, 2007b). \(^c\) Quantity of benzo(a)pyrene. \(^d\) The Swedish Medical Products Agency (MPA). \(^e\) Swedish Chemical Agency (2006). \(^f\) Quantity of 1,2-dichlorobenzene. \(^g\) Lindberg et al. (2005). \(^h\) Quantity of PBDE 209. \(^i\) demeclocycline and chlorotetracycline not included. \(^j\) In Sweden.
<table>
<thead>
<tr>
<th>Class of compound</th>
<th>Sub group</th>
<th>M_w (g mol⁻¹)ᵃ</th>
<th>log K_owᵇ</th>
<th>S_w (mg L⁻¹)ᶜ</th>
<th>H (atm·m³ mol⁻³)ᵈ</th>
</tr>
</thead>
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<td>Metals</td>
<td>As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn</td>
<td>51 - 207</td>
<td>-0.6 - 0.7</td>
<td>6·10⁻⁴ - 4·10⁵</td>
<td>2·10⁻² - 0.8</td>
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<tr>
<td>Esters</td>
<td>Phthalates</td>
<td>194 - 447</td>
<td>1.7 - 10</td>
<td>1·10⁻⁵ - 8·10⁴</td>
<td>4·10⁻⁸ - 4·10⁻⁵</td>
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<td>Adipates</td>
<td>202 - 427</td>
<td>2.4 - 10</td>
<td>4·10⁻⁶ - 690</td>
<td>2·10⁻⁶ - 2·10⁻⁴</td>
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<td></td>
<td>OPs</td>
<td>266 - 431</td>
<td>1.6 - 4.7</td>
<td>5·6 - 10³</td>
<td>1·10⁻¹¹ - 3·10⁻⁶</td>
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<tr>
<td>Pesticides</td>
<td>Biocides</td>
<td>110 - 362</td>
<td>1 - 4.7</td>
<td>7·10⁻⁶ - 3·10⁵</td>
<td>6·10⁻¹² - 5·10⁻⁷</td>
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<td></td>
<td>Insecticides</td>
<td>183 - 505</td>
<td>-0.9 - 7.4</td>
<td>2·10⁻³ - 1·10⁶</td>
<td>3·10⁻¹² - 4·10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>Herbicides</td>
<td>111 - 412</td>
<td>-4.5 - 5.3</td>
<td>5·10⁻² - 1·10⁶</td>
<td>4·10⁻¹⁹ - 2·10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>Fungicides</td>
<td>169 - 403</td>
<td>0.9 - 5.5</td>
<td>4·10⁻² - 9·10³</td>
<td>8·10⁻¹⁴ - 3·10⁻⁵</td>
</tr>
<tr>
<td>Hydrocarbons</td>
<td>PAHs</td>
<td>202 - 276</td>
<td>4.9 - 6.7</td>
<td>2·10⁻⁴ - 9·10⁻²</td>
<td>1·10⁻⁷ - 8·10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>Terpene (Limonene)</td>
<td>136</td>
<td>4.8</td>
<td>44</td>
<td>0.4</td>
</tr>
<tr>
<td>Phenols</td>
<td>Chlorophenols</td>
<td>129 - 266</td>
<td>2.2 - 4.7</td>
<td>45 - 1·10⁴</td>
<td>1·10⁻⁷ - 4·10⁻⁷</td>
</tr>
<tr>
<td></td>
<td>Butylhydroxytoluene</td>
<td>220</td>
<td>5.0</td>
<td>10</td>
<td>4·10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>Triclosan</td>
<td>290</td>
<td>4.7</td>
<td>9.3</td>
<td>5·10⁻⁹</td>
</tr>
<tr>
<td></td>
<td>4-Nonylphenol</td>
<td>220</td>
<td>5.9</td>
<td>2.7</td>
<td>6·10⁻⁶</td>
</tr>
<tr>
<td>Organometals</td>
<td>Organotin compounds</td>
<td>177 - 351</td>
<td>0.6 - 7.4</td>
<td>6·10⁻⁷ - 4·10³</td>
<td>1·10⁻⁹ - 1.5</td>
</tr>
<tr>
<td>Pharmaceuticals</td>
<td>Fluoroquinolones</td>
<td>319 - 361</td>
<td>-0.3 - 0.3⁸</td>
<td>7·10⁻⁷ - 4·10⁴</td>
<td>5·10⁻²⁰ - 9·10⁻¹⁹</td>
</tr>
<tr>
<td></td>
<td>Tetracyclines</td>
<td>444 - 483</td>
<td>-4 - -0.7</td>
<td>160 - 3·10⁵</td>
<td>1·10⁻¹¹ - 5·10⁻²⁴</td>
</tr>
<tr>
<td></td>
<td>NSAIDs</td>
<td>206 - 296</td>
<td>3.0 - 4.0</td>
<td>11 - 260</td>
<td>5·10⁻¹² - 2·10⁻⁷</td>
</tr>
<tr>
<td></td>
<td>Hormones</td>
<td>272 - 298</td>
<td>2.8 - 4.1</td>
<td>13 - 560</td>
<td>1·10⁻¹² - 6·10⁻¹⁰</td>
</tr>
<tr>
<td>Siloxanes</td>
<td>Methylsiloxanes</td>
<td>162 - 445</td>
<td>4.8 - 6.5</td>
<td>1·10⁻⁴ - 1.4</td>
<td>9·10⁻² - 0.8</td>
</tr>
<tr>
<td>Fluorinated compounds</td>
<td>Perfluorochemicals</td>
<td>314 - 714</td>
<td>2.2 - 12</td>
<td>6·10⁻⁷ - 2</td>
<td>1·10⁻⁹ - 2·10⁻⁴</td>
</tr>
<tr>
<td>Halogenated compounds</td>
<td>Polychlorobenzenes</td>
<td>147 - 285</td>
<td>3.3 - 5.9</td>
<td>0.3 - 100</td>
<td>9·10⁻⁴ - 3·10⁻³</td>
</tr>
<tr>
<td></td>
<td>PBDEs</td>
<td>407 - 959</td>
<td>5.9 - 12</td>
<td>3·10⁻⁶ - 0.3</td>
<td>1·10⁻⁸ - 7·10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>I-PCBs</td>
<td>258 - 395</td>
<td>5.7 - 8.3</td>
<td>4·10⁻⁴ - 0.1</td>
<td>5·10⁻⁵ - 2·10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>WHO-PCBs</td>
<td>292 - 395</td>
<td>6.3 - 8.3</td>
<td>4·10⁻⁴ - 3·10⁻²</td>
<td>5·10⁻⁵ - 1·10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>PCDD/Fs</td>
<td>306 - 460</td>
<td>6.3 - 9.5</td>
<td>9·10⁻⁶ - 3·10⁻²</td>
<td>1·10⁻⁶ - 2·10⁻⁵</td>
</tr>
</tbody>
</table>

Abbreviations can be found in Table 1. Mₜ: Molecular weight. log K_ow: octanol-water partition coefficient, estimated values. Sₜ: Water solubility, estimated values. H: Henry’s Law Constant, estimated values. ⁵Experimentally determined value (Takacs-Novak et al., 1992).
Table 3 Descriptive data of the investigated sewage treatment plants (STPs) (STPs, 2005)

<table>
<thead>
<tr>
<th>STP ID</th>
<th>Stockholm A</th>
<th>Gothenburg B</th>
<th>Eslöv C</th>
<th>Umeå D</th>
<th>Borås E</th>
<th>Alingsås F</th>
<th>Floda G</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inhabitants served</td>
<td>684 000</td>
<td>621 000</td>
<td>17 500</td>
<td>84 000</td>
<td>79 000</td>
<td>24 000</td>
<td>10 000</td>
</tr>
<tr>
<td>No. of personal equivalents (pe)</td>
<td>835 000</td>
<td>772 000</td>
<td>100 000</td>
<td>100 000</td>
<td>98 000</td>
<td>37 000</td>
<td>6 000</td>
</tr>
<tr>
<td>Dimensioning of the STP (pe)</td>
<td>900 000</td>
<td>680 000</td>
<td>330 000</td>
<td>116 000</td>
<td>110 000</td>
<td>60 000</td>
<td>13 000</td>
</tr>
<tr>
<td>Type of activity connected</td>
<td>Ind. (mix)</td>
<td>Ind. (mix)</td>
<td>Ind. (F)</td>
<td>H</td>
<td>H/Ind. (T, C)</td>
<td>Ind. (L)</td>
<td>House</td>
</tr>
<tr>
<td>Treatment of the sewage</td>
<td>M/C/B/D</td>
<td>M/C/B/D</td>
<td>M/B/C/D</td>
<td>M/C/B/D</td>
<td>M/C/B/D</td>
<td>M/C/B/D</td>
<td>M/C/B/S</td>
</tr>
<tr>
<td>Solid t, (days)</td>
<td>15</td>
<td>15</td>
<td>30</td>
<td>18</td>
<td>29</td>
<td>17</td>
<td>18</td>
</tr>
<tr>
<td>Raw sewage water (Mm$^3$ year$^{-1}$)</td>
<td>88</td>
<td>117</td>
<td>4.6</td>
<td>12</td>
<td>18</td>
<td>4.6</td>
<td>1.5</td>
</tr>
<tr>
<td>Storm water (%)</td>
<td>5</td>
<td>50</td>
<td>43</td>
<td>20</td>
<td>59</td>
<td>38</td>
<td>66</td>
</tr>
<tr>
<td>Sewage sludge (tonnes d.w. year$^{-1}$)</td>
<td>14 300</td>
<td>13 500</td>
<td>1 600</td>
<td>2 300</td>
<td>3 500</td>
<td>770</td>
<td>270</td>
</tr>
<tr>
<td>Fraction of total production (%)</td>
<td>6.0</td>
<td>5.6</td>
<td>0.67</td>
<td>1.0</td>
<td>1.5</td>
<td>0.32</td>
<td>0.11</td>
</tr>
<tr>
<td>Sewage sludge d.w. (%)</td>
<td>29</td>
<td>28</td>
<td>21</td>
<td>37</td>
<td>22</td>
<td>23</td>
<td>30</td>
</tr>
</tbody>
</table>

$^a$Ind., industry; mix, mixture of industrial sewage; F, food; H, hospital; T, textile; C, chemical; L, laundry; and House, household. $^b$M, mechanical; C, chemical; B, biological treatment (activated sludge); D, digestion (anaerobic); and S, stabilization (aerobic) of the sludge. $^c$Solid retention time in the digester/aerobic stabilizer. $^d$Percentage of the total annual production of sewage sludge in Sweden (Swedish EPA, 2007). $^e$Percent dry weight of total mass.
Table 4 Detection frequencies (Det. Freq.), concentration ranges, measured concentrations (MC), mass flows (MF), and percentage of the compounds found (recovered) in the sewage sludge relative the amounts used

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Det. Freq.</th>
<th>Measured concentrations (MC)</th>
<th>MF (kg year(^{-1}))</th>
<th>Rec. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>min</td>
<td>max</td>
<td>average</td>
</tr>
<tr>
<td>As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn</td>
<td>7/7</td>
<td>500 000</td>
<td>1 100 000</td>
<td>800 000</td>
</tr>
<tr>
<td>Phthalates</td>
<td>7/7</td>
<td>69 000</td>
<td>320 000</td>
<td>120 000</td>
</tr>
<tr>
<td>Polychlorinated alkanes (PCAs)</td>
<td>7/7</td>
<td>9 900</td>
<td>82 000</td>
<td>50 000</td>
</tr>
<tr>
<td>Siloxanes</td>
<td>3/3</td>
<td>13 000</td>
<td>25 000</td>
<td>22 000</td>
</tr>
<tr>
<td>Biocides</td>
<td>7/7</td>
<td>4 000</td>
<td>62 000</td>
<td>14 000</td>
</tr>
<tr>
<td>4-Nonylphenol</td>
<td>7/7</td>
<td>8 000</td>
<td>40 000</td>
<td>13 000</td>
</tr>
<tr>
<td>Fluoroquinolones (FQs)</td>
<td>7/7</td>
<td>7 000</td>
<td>16 000</td>
<td>13 000</td>
</tr>
<tr>
<td>Triclosan</td>
<td>7/7</td>
<td>1 800</td>
<td>8 300</td>
<td>3 700</td>
</tr>
<tr>
<td>Tetracyclines (TCs)</td>
<td>2/2</td>
<td>1 400</td>
<td>4 100</td>
<td>2 800</td>
</tr>
<tr>
<td>Pesticides</td>
<td>4/7</td>
<td>2 100</td>
<td>10 000</td>
<td>2 100</td>
</tr>
<tr>
<td>Butylhydroxytoluene (BHT)</td>
<td>7/7</td>
<td>640</td>
<td>2 400</td>
<td>1 500</td>
</tr>
<tr>
<td>Organophosphorus compounds (OPs)</td>
<td>7/7</td>
<td>310</td>
<td>2 800</td>
<td>730</td>
</tr>
<tr>
<td>Polycyclic aromatic hydrocarbons (PAHs)</td>
<td>6/7</td>
<td>470</td>
<td>1 700</td>
<td>640</td>
</tr>
<tr>
<td>Polychlorinated diphenylethers (PBDEs)</td>
<td>7/7</td>
<td>390</td>
<td>870</td>
<td>550</td>
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<tr>
<td>Organotin compounds (OTCs)</td>
<td>7/7</td>
<td>230</td>
<td>480</td>
<td>410</td>
</tr>
<tr>
<td>Terpene (Limonene)</td>
<td>2/2</td>
<td>150</td>
<td>500</td>
<td>330</td>
</tr>
<tr>
<td>Non-steroid anti-inflammatory drugs (NSAIDs)</td>
<td>2/2</td>
<td>62</td>
<td>230</td>
<td>140</td>
</tr>
<tr>
<td>Chlorophenols (CPs)</td>
<td>6/7</td>
<td>34</td>
<td>130</td>
<td>92</td>
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<tr>
<td>Adipates</td>
<td>2/2</td>
<td>40</td>
<td>100</td>
<td>70</td>
</tr>
<tr>
<td>Indicator-PCBs</td>
<td>7/7</td>
<td>23</td>
<td>100</td>
<td>50</td>
</tr>
<tr>
<td>Polychlorobenzenes</td>
<td>7/7</td>
<td>20</td>
<td>330</td>
<td>39</td>
</tr>
<tr>
<td>Perfluorochemicals (PFCs)</td>
<td>7/7</td>
<td>13</td>
<td>290</td>
<td>38</td>
</tr>
<tr>
<td>WHO-PCBs</td>
<td>7/7</td>
<td>3.2</td>
<td>11</td>
<td>6</td>
</tr>
<tr>
<td>Polychlorinated dioxins/furans (PCDD/Fs)</td>
<td>7/7</td>
<td>0.96</td>
<td>2.2</td>
<td>1.6</td>
</tr>
<tr>
<td>Hormones</td>
<td>0/2</td>
<td>&lt;LoD(^e)</td>
<td>&lt;LoD(^e)</td>
<td>&lt;LoD(^e)</td>
</tr>
</tbody>
</table>

\(^a\)Number of positive samples/number of STPs. \(^b\)RSD: Relative Standard Deviation. \(^c\)MF: Mass Flow, based on MC and the annual production of sewage sludge (Swedish EPA, 2007). \(^d\)Percentage of the compounds recovered in sewage sludge, of the annual quantity recorded in Sweden in 2004 (Swedish Chemicals Agency, 2007b). \(^e\)LoD: Limit-of-Detection.
Fig. 1. Median total concentrations (logarithmic scale) of each measured group of metals, persistent organic pollutants, pharmaceuticals and personal care products, and other organic contaminants in sludge from sewage treatment plants (STPs) in Sweden. The error bars correspond to the ranges of total concentrations (n=7 STPs, unless otherwise indicated). Abbreviations: PCAs, Polychlorinated alkanes; FQs, Fluoroquinolones; 4-NP, 4-nonylphenol; TCs, Tetracyclines; BHT, Butylhydroxytoluene; OPs, Organophosphorus compounds; PAHs, Polycyclic aromatic hydrocarbons; PBDEs, Polybrominated diphenylethers; OTCs, Organotin compounds; NSAIDs, Non-steroid anti-inflammatory drugs; CPs, Chlorophenols; I-PCBs, Indicator-PCBs; PCBz, Polychlorobenzenes; PFCs, Perfluorochemicals; PCDD/Fs, Polychlorinated dibenzo-\(p\)-dioxins and -furans.
Fig. 2. Molecular weight ($M_w$ g mol$^{-1}$) vs. percentage recovered (%) in sludge of plastic additives (plasticizers and/or flame retardants), $R^2=0.94$ (TCPP excluded). OPs, organophosphorus compounds (TBP, tributyl phosphate; TCEP, tris(2-chloroethyl) phosphate; TPP, triphenyl phosphate; TCPP, tris(2-chloroisopropyl) phosphate; TDCPP, tris(1,3-dichloro-2-propyl) phosphate); DEHA, di-(2-ethylhexyl) adipate; Phthalates (DEHP, di-(2-ethylhexyl) phthalate; DINP, di-iso-nonyl phthalate; DIDP, di-iso-decyl phthalate); PBDE #209, decabrominated diphenylether.
Fig. 3. Principal Component Analysis (PCA) plots displaying patterns in levels of contaminants in sewage at the selected sewage treatment plants (STPs), based on measured concentrations of the compounds analyzed in all STPs (n=7), with levels below the limit-of-detection, LoD, were set to half the LoD. The first and second principal components (PC1 and PC2) explained 34% and 21%, respectively, of the total variance in the data. a: score plot showing relationships between the Swedish STPs. b-e: loading plots showing the corresponding relationships among the metals, persistent organic pollutants, pharmaceuticals and personal care products, and other organic contaminants. For compound abbreviations, see Table S1. The three congested areas (boxes with broken lines) include: PFDoA, PFDA, PFUnA, PFNA, PFTiDA, PFTeDA, PFHpA (panel b); ETPARAB, BUPARAB, BEPARAB, RESORCINOL, PROPARAB (panel c); and 1234789-CDD, 1234678-CDF, 123678-CDD, 2378-CDF, MCCP, OCDF, 14CBz, HCBz (panel d).
Supplementary data

Comprehensive mass flow analysis of Swedish sludge contaminants
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Figures: 2
Tables: 3
Selection of chemicals

The organic compounds monitored in the Swedish annual sludge sampling program, and included in this study, were selected from Scandinavian priority lists, the European Union Water Framework Directive (WFD) (EU, 2000), or the “Working document on sludge” (CEC, 2000). A wide range of biocides and pesticides are also included (generated from the Swedish EPA emerging pollutants screening program), most of which are restricted in the EU (EU, 1991) and classified as POPs (UNEP, 2001) or as WFD priority substances (EU, 2000). As part of their normal routines the STPs monitor levels of polycyclic aromatic hydrocarbons (PAHs), PCBs, and 4-nonylphenol (compiled from environmental reports).

Sewage treatment plants and sample collection

Dewatered digested (anaerobic) or stabilized (aerobic) sludge was collected at seven STPs (Table 3 and Fig. S1) spread across Sweden in the autumn of 2004 (unless otherwise stated). These STPs represent large-, medium- and small-sized plants. Samples were collected during periods of normal working and weather conditions. Composite samples (n=3) from each STP were collected in dark bottles within one hour after sludge dewatering. In order to reduce the risk of microbial degradation, the sludge samples were frozen immediately after sampling and stored in freezer at -18°C until the chemical analysis.

Analysis and QA/QC

The chemical analyses were performed at Swedish laboratories experienced in the analysis of the target substances. These laboratories use established laboratory quality assurance and quality control (QA/QC) procedures. In parallel with all samples, method blank samples were run as controls to ensure that any contamination during preparation, clean-up, and instrumental analysis did not significantly influence the quantitative results. For a positive identification the analyte chromatographic retention time had to agree with that of an authentic reference standard and its signal intensity had to be at least 3×LoD (limit-of-detection).
Fig. S1. Map of sampling locations in Sweden, STPs A-G; A, Stockholm; B, Gothenburg; C, Eslöv; D, Umeå; E, Borås; F, Alingsås; G, Floda.
Fig. S2. Distribution patterns and total concentrations of the perfluorochemicals (PFCs), and fractions of the total occurrences of PFCs detected in sludge from the sewage treatment plants (STPs A-G; A, Stockholm; B, Gothenburg; C, Eslöv; D, Umeå; E, Borås; F, Alingsås; G, Floda) in Sweden.

Abbreviations:
PFHxA, perfluorohexane acid; PFHxS, perfluorohexane sulfonate; PFHpA, perfluoroheptane acid; PFOA, perfluorooctanoic acid; PFNA, perfluorononanoic acid; PFOS, perfluorooctane sulfonate; PFOSA, perfluorooctane sulfonamide; PFDA, perfluorodecanoic acid; PFUnA, perfluoroundecanoic acid; PFDS, perfluorodecanesulfonate; PFDoA, perfluorododecanoic acid; PFTDA, perfluorotridecanoic acid and PFTeDA, perfluorotetradecanoic acid.
**Table S1.** CAS numbers and chemical and physical properties of the metals, persistent organic pollutants (POPs), pharmaceuticals, and other organic contaminants (EPI Suite™, 2007)

*Priority substance included in the WFD (EU, 2000), **classified as POP according to the Stockholm Convention (UNEP, 2001), n.e., not estimated, abbreviations of the compounds used in the PCA model are presented in parenthesis.

<table>
<thead>
<tr>
<th>Chemical</th>
<th>CAS RN&lt;sup&gt;a&lt;/sup&gt;</th>
<th>M&lt;sub&gt;w&lt;/sub&gt; (g mol&lt;sup&gt;−1&lt;/sup&gt;)</th>
<th>log K&lt;sub&gt;ow&lt;/sub&gt;&lt;sup&gt;c&lt;/sup&gt;</th>
<th>S&lt;sub&gt;w&lt;/sub&gt; (mg L&lt;sup&gt;−1&lt;/sup&gt;)&lt;sup&gt;d&lt;/sup&gt;</th>
<th>Henry’s Law Constant&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Phenols</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorophenols (CPs)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-monochlorophenol (2-CP)</td>
<td>95-57-8</td>
<td>128.56</td>
<td>2.16</td>
<td>12 734</td>
<td>4.2·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>3-monochlorophenol (3-CP)</td>
<td>108-43-0</td>
<td>128.56</td>
<td>2.16</td>
<td>12 734</td>
<td>4.2·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>4-monochlorophenol (4-CP)</td>
<td>106-48-9</td>
<td>128.56</td>
<td>2.16</td>
<td>12 734</td>
<td>4.2·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,3-dichlorophenol (23-CP)</td>
<td>576-24-9</td>
<td>163.00</td>
<td>2.80</td>
<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,4-dichlorophenol (24-CP)</td>
<td>120-83-2</td>
<td>163.00</td>
<td>2.80</td>
<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,5-dichlorophenol (25-CP)</td>
<td>583-78-8</td>
<td>163.00</td>
<td>2.80</td>
<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,6-dichlorophenol (26-CP)</td>
<td>87-65-0</td>
<td>163.00</td>
<td>2.80</td>
<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>3,4-dichlorophenol (34-CP)</td>
<td>95-77-2</td>
<td>163.00</td>
<td>2.80</td>
<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>3,5-dichlorophenol (35-CP)</td>
<td>591-35-5</td>
<td>163.00</td>
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<td>3 282</td>
<td>3.1·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<td>2,3,4-trichlorophenol (234-CP)</td>
<td>15950-66-0</td>
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<td>3.45</td>
<td>808</td>
<td>2.3·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>2,3,5-trichlorophenol (235-CP)</td>
<td>933-78-8</td>
<td>197.45</td>
<td>3.45</td>
<td>808</td>
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<td>2,3,6-trichlorophenol (236-CP)</td>
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<td>2,4,5-trichlorophenol (245-CP)</td>
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<td>197.45</td>
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<tr>
<td>3,4,5-trichlorophenol (345-CP)</td>
<td>609-19-8</td>
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<td>3.45</td>
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<td>2.3·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>2,3,4,5-tetrachlorophenol (2345-CP)</td>
<td>4901-51-3</td>
<td>231.89</td>
<td>4.09</td>
<td>193</td>
<td>1.7·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>2,3,4,6-tetrachlorophenol (2346-CP)</td>
<td>58-90-2</td>
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<td>193</td>
<td>1.7·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>2,3,5,6-tetrachlorophenol (2356-CP)</td>
<td>935-95-5</td>
<td>231.89</td>
<td>4.09</td>
<td>193</td>
<td>1.7·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>Pentachlorophenol* (PCP)</td>
<td>87-86-5</td>
<td>266.34</td>
<td>4.74</td>
<td>45</td>
<td>1.3·10&lt;sup&gt;7&lt;/sup&gt;</td>
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<tr>
<td>4-Nonylphenol* (4NP)</td>
<td>84852-15-3</td>
<td>220.36</td>
<td>5.92</td>
<td>2.7</td>
<td>6.0·10&lt;sup&gt;6&lt;/sup&gt;</td>
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<td>Butylhydroxytoluene (BHT)</td>
<td>128-37-0</td>
<td>220.36</td>
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<td>10</td>
<td>4.1·10&lt;sup&gt;6&lt;/sup&gt;</td>
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<td>Triclosan (TCS)</td>
<td>3380-34-5</td>
<td>289.55</td>
<td>4.66</td>
<td>9.3</td>
<td>5.0·10&lt;sup&gt;9&lt;/sup&gt;</td>
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<td><strong>Chlorobenzenes</strong></td>
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<td>1,2-dichlorobenzene (12CBz)</td>
<td>95-50-1</td>
<td>147.00</td>
<td>3.28</td>
<td>104</td>
<td>3.0·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,3-dichlorobenzene (13CBz)</td>
<td>541-73-1</td>
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<td>3.28</td>
<td>104</td>
<td>3.0·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,4-dichlorobenzene (14CBz)</td>
<td>106-46-7</td>
<td>147.00</td>
<td>3.28</td>
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<td>3.0·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,2,3-trichlorobenzene* (123CBz)</td>
<td>87-61-6</td>
<td>181.45</td>
<td>3.93</td>
<td>26</td>
<td>2.2·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,2,4-trichlorobenzene* (124CBz)</td>
<td>120-82-1</td>
<td>181.45</td>
<td>3.93</td>
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<td>2.2·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<td>1,3,5-trichlorobenzene* (135CBz)</td>
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<td>3.93</td>
<td>26</td>
<td>2.2·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,2,3,4-tetrachlorobenzene (1234CBz)</td>
<td>634-66-2</td>
<td>215.89</td>
<td>4.57</td>
<td>6.3</td>
<td>1.6·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>1,2,3,5-tetrachlorobenzene (1235CBz)</td>
<td>634-90-2</td>
<td>215.89</td>
<td>4.57</td>
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<td>1,2,4,5-tetrachlorobenzene (1245CBz)</td>
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<td>6.3</td>
<td>1.6·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>Pentachlorobenzene* ** (PCBz)</td>
<td>608-93-5</td>
<td>250.34</td>
<td>5.22</td>
<td>1.5</td>
<td>1.2·10&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>Hexachlorobenzene* ** (HCBz)</td>
<td>118-74-1</td>
<td>284.78</td>
<td>5.86</td>
<td>0.3</td>
<td>8.9·10&lt;sup&gt;4&lt;/sup&gt;</td>
</tr>
<tr>
<td><strong>Esters</strong></td>
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S5
### Organophosphorus compounds (OPs)

<table>
<thead>
<tr>
<th>Compound</th>
<th>LogP</th>
<th>MW</th>
<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
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<tbody>
<tr>
<td>Tributyl phosphate (TBP)</td>
<td>126-73-8</td>
<td>266.32</td>
<td>3.82</td>
<td>101</td>
<td>3.2·10^{-6}</td>
</tr>
<tr>
<td>Triphenyl phosphate (TPP)</td>
<td>115-86-6</td>
<td>326.29</td>
<td>4.70</td>
<td>47</td>
<td>4.0·10^{-8}</td>
</tr>
<tr>
<td>Tris(2-chloroethyl) phosphate (TCEP)</td>
<td>115-96-8</td>
<td>285.49</td>
<td>1.63</td>
<td>597</td>
<td>2.6·10^{-8}</td>
</tr>
<tr>
<td>Tris(2-chloroisopropyl) phosphate (TCP)</td>
<td>13674-84-5</td>
<td>327.57</td>
<td>2.89</td>
<td>740</td>
<td>6.0·10^{-8}</td>
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<tr>
<td>Tris(1,3-dichloro-2-propyl) phosphate (TDCP)</td>
<td>13674-87-8</td>
<td>430.91</td>
<td>3.65</td>
<td>30</td>
<td>2.6·10^{-9}</td>
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<tr>
<td>Tris(2-butoxyethyl) phosphate (TBEP)</td>
<td>78-51-3</td>
<td>398.48</td>
<td>3.00</td>
<td>604</td>
<td>1.2·10^{-11}</td>
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### Phthalates

<table>
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<tr>
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<th>LogP</th>
<th>MW</th>
<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimethyl phthalate (DMP)</td>
<td>131-11-3</td>
<td>194.19</td>
<td>1.66</td>
<td>7459</td>
<td>2.2·10^{-7}</td>
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<tr>
<td>Diethyl phthalate (DEP)</td>
<td>84-66-2</td>
<td>222.24</td>
<td>2.65</td>
<td>720</td>
<td>3.9·10^{-7}</td>
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<tr>
<td>Di-n-butyl phthalate (DBP)</td>
<td>84-74-2</td>
<td>278.35</td>
<td>4.61</td>
<td>6.4</td>
<td>1.2·10^{-6}</td>
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<tr>
<td>Butylbenzyl phthalate (BBP)</td>
<td>85-68-7</td>
<td>312.37</td>
<td>4.84</td>
<td>1.1</td>
<td>4.2·10^{-8}</td>
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<tr>
<td>Di-(2-ethylhexyl) phthalate (DEHP)*</td>
<td>117-81-7</td>
<td>390.57</td>
<td>8.39</td>
<td>1.3·10^{-3}</td>
<td>1.2·10^{-5}</td>
</tr>
<tr>
<td>Di-n-octyl phthalate (DNOP)</td>
<td>117-84-0</td>
<td>390.57</td>
<td>8.54</td>
<td>4.5·10^{-3}</td>
<td>1.2·10^{-5}</td>
</tr>
<tr>
<td>Di-octyl phthalate (DIDP)</td>
<td>68515-49-1</td>
<td>446.68</td>
<td>10.36</td>
<td>1.0·10^{-5}</td>
<td>3.7·10^{-5}</td>
</tr>
<tr>
<td>Di-octyl phthalate (DINP)</td>
<td>28553-12-0</td>
<td>418.62</td>
<td>9.37</td>
<td>1.2·10^{-4}</td>
<td>2.1·10^{-5}</td>
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**Adipates (not included in the PCA model)**

<table>
<thead>
<tr>
<th>Compound</th>
<th>LogP</th>
<th>MW</th>
<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
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<tr>
<td>Diethyl adipate</td>
<td>141-28-6</td>
<td>202.25</td>
<td>2.37</td>
<td>695</td>
<td>1.7·10^{-6}</td>
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<tr>
<td>Di-octyl adipate</td>
<td>141-04-8</td>
<td>258.36</td>
<td>4.19</td>
<td>18</td>
<td>5.4·10^{-6}</td>
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<tr>
<td>Dibutyl adipate</td>
<td>105-99-7</td>
<td>258.36</td>
<td>4.33</td>
<td>6.31</td>
<td>5.4·10^{-6}</td>
</tr>
<tr>
<td>Di(2-ethylhexyl) adipate</td>
<td>103-23-1</td>
<td>370.58</td>
<td>8.12</td>
<td>1.3·10^{-3}</td>
<td>5.2·10^{-5}</td>
</tr>
<tr>
<td>Diocyl adipate</td>
<td>123-79-5</td>
<td>370.58</td>
<td>8.26</td>
<td>4.6·10^{-3}</td>
<td>5.2·10^{-5}</td>
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<tr>
<td>Didecyl adipate</td>
<td>105-97-5</td>
<td>426.69</td>
<td>10.23</td>
<td>3.8·10^{-6}</td>
<td>1.6·10^{-4}</td>
</tr>
<tr>
<td>Di-octyl adipate</td>
<td>1330-86-5</td>
<td>370.58</td>
<td>8.12</td>
<td>1.3·10^{-3}</td>
<td>5.2·10^{-5}</td>
</tr>
<tr>
<td>Di-decyl adipate</td>
<td>27178-16-1</td>
<td>426.69</td>
<td>10.08</td>
<td>1.1·10^{-5}</td>
<td>1.6·10^{-4}</td>
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### Antibiotics

#### Fluoroquinolones (FQs)

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<th>MW</th>
<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
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</thead>
<tbody>
<tr>
<td>Norfloxacin (Nor)</td>
<td>70458-96-7</td>
<td>319.34</td>
<td>-0.31</td>
<td>40231</td>
<td>8.7·10^{-19}</td>
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<tr>
<td>Ofloxacin (Ofl)</td>
<td>82419-36-1</td>
<td>361.38</td>
<td>-0.20</td>
<td>6873</td>
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<td>Ciprofloxacin (Cip)</td>
<td>85721-33-1</td>
<td>331.35</td>
<td>0.28</td>
<td>19440</td>
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#### Tetracyclines (not included in the PCA model)

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<th>LogP</th>
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<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
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<tr>
<td>Oxytetracycline</td>
<td>2058-46-0</td>
<td>450.88</td>
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<td>156</td>
<td>1.7·10^{-9}</td>
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<tr>
<td>Tetracycline</td>
<td>64-75-5</td>
<td>482.92</td>
<td>-3.70</td>
<td>3.4·10^{-5}</td>
<td>1.3·10^{-11}</td>
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<tr>
<td>Demeclocycline</td>
<td>127-33-3</td>
<td>464.86</td>
<td>-1.14</td>
<td>8.6·10^{-4}</td>
<td>2.6·10^{-14}</td>
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<tr>
<td>Chlorotetracycline</td>
<td>57-62-5</td>
<td>478.89</td>
<td>-0.68</td>
<td>3.8·10^{-4}</td>
<td>3.5·10^{-24}</td>
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<td>Doxycycline</td>
<td>564-25-0</td>
<td>444.44</td>
<td>-1.36</td>
<td>1.2·10^{-5}</td>
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### Pharmaceuticals (not included in the PCA model)

#### Non-steroid anti-inflammatory drugs (NSAIDs)

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<th>ClogP</th>
<th>EC50</th>
<th>P50</th>
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<tr>
<td>Ibuprofen</td>
<td>15687-27-1</td>
<td>206.29</td>
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<tr>
<td>Naproxen</td>
<td>22204-53-1</td>
<td>230.27</td>
<td>3.10</td>
<td>44</td>
<td>3.4·10^{-10}</td>
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<tr>
<td>Ketoprofen</td>
<td>22071-15-4</td>
<td>254.29</td>
<td>3.00</td>
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<td>2.1·10^{-11}</td>
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<td>Diclofenac</td>
<td>15307-86-5</td>
<td>296.15</td>
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**Hormones**

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<th>Hormone</th>
<th>Mass (amu)</th>
<th>Abundance (aM)</th>
<th>Binding (aM)</th>
<th>Plasma Protein Binding (%)</th>
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<tbody>
<tr>
<td>Estriol</td>
<td>50-27-1</td>
<td>288.39</td>
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<td>Estradiol</td>
<td>50-28-2</td>
<td>272.39</td>
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<tr>
<td>Ethinylestradiol</td>
<td>57-63-6</td>
<td>296.41</td>
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<tr>
<td>Norethindrone</td>
<td>68-22-4</td>
<td>284.43</td>
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**Dioxin-like compounds**

**Polychlorinated biphenyls (WHO-PCBs)**

<table>
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<th>Mass (amu)</th>
<th>Abundance (aM)</th>
<th>Binding (aM)</th>
<th>Plasma Protein Binding (%)</th>
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<tbody>
<tr>
<td>PCB 77</td>
<td>32598-13-3</td>
<td>291.99</td>
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<td>70362-50-4</td>
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<td>6.34</td>
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<td>PCB 126</td>
<td>57465-28-8</td>
<td>326.44</td>
<td>6.98</td>
<td>7.3·10⁻³</td>
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<tr>
<td>PCB 169</td>
<td>32774-16-6</td>
<td>360.88</td>
<td>7.62</td>
<td>1.6·10⁻⁵</td>
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<td>32598-14-4</td>
<td>326.44</td>
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<td>74472-37-0</td>
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<td>PCB 156</td>
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<td>7.62</td>
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<td>7.62</td>
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<tr>
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<td>PCB 189</td>
<td>39635-31-9</td>
<td>395.33</td>
<td>8.27</td>
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**Polychlorinated dibenzo-p-dioxins and -furans (PCDD/Fs)**

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<th>Compound</th>
<th>Mass (amu)</th>
<th>Abundance (aM)</th>
<th>Binding (aM)</th>
<th>Plasma Protein Binding (%)</th>
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</thead>
<tbody>
<tr>
<td>2,3,7,8-TCDD (2378-CDD)</td>
<td>1746-01-6</td>
<td>321.98</td>
<td>6.92</td>
<td>3·10⁻³</td>
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<tr>
<td>1,2,3,7,8-PeCDD (12378-CDD)</td>
<td>40321-76-4</td>
<td>356.42</td>
<td>7.56</td>
<td>8·10⁻⁴</td>
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<tr>
<td>1,2,3,4,7,8-HxCDD (123478-CDD)</td>
<td>39227-28-6</td>
<td>390.87</td>
<td>8.21</td>
<td>1·10⁻³</td>
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<td>1,2,3,6,7,8-HxCDD (123678-CDD)</td>
<td>57653-85-7</td>
<td>390.87</td>
<td>8.21</td>
<td>1·10⁻³</td>
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<td>1,2,3,7,8,9-HxCDD (123789-CDD)</td>
<td>19408-74-3</td>
<td>390.87</td>
<td>8.21</td>
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<td>1,2,3,4,6,7,8-HpCDD (1234678-CDD)</td>
<td>35822-46-9</td>
<td>425.31</td>
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<td>4·10⁻⁵</td>
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<td>OCDD</td>
<td>3268-87-9</td>
<td>459.76</td>
<td>9.50</td>
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<td>2,3,7,8-TCDF (2378-CDF)</td>
<td>51207-31-9</td>
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<td>1,2,3,7,8-PeCDF (12378-CDF)</td>
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<td>6·10⁻⁵</td>
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<td>1,2,3,4,7,8-HxCDF (123478-CDF)</td>
<td>70648-26-9</td>
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<td>1,2,3,6,7,8-HxCDF (123678-CDF)</td>
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<td>2,3,4,6,7,8-HxCDF (234678-CDF)</td>
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<td>1,2,3,7,8,9-HxCDF (123789-CDF)</td>
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<td>1,2,3,4,6,7,8-HpCDF (1234678-CDF)</td>
<td>67562-39-4</td>
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<td>1,2,3,4,7,8,9-HpCDF (1234789-CDF)</td>
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### Other organic compounds

**Polycyclic aromatic hydrocarbons**

*(PAHs)* (PAHsum)

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<th>$9.1 \times 10^{-2}$</th>
<th>$8.3 \times 10^{-6}$</th>
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<tbody>
<tr>
<td>Fluoranthene</td>
<td>205-99-2</td>
<td>252.32</td>
<td>6.11</td>
<td>$2.0 \times 10^{-3}$</td>
<td>$8.1 \times 10^{-7}$</td>
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<tr>
<td>Benzo(b)fluoranthene</td>
<td>207-08-9</td>
<td>252.32</td>
<td>6.11</td>
<td>$2.0 \times 10^{-3}$</td>
<td>$8.1 \times 10^{-7}$</td>
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<tr>
<td>Benzo(k)fluoranthene</td>
<td>50-32-8</td>
<td>252.32</td>
<td>6.11</td>
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<td>$8.1 \times 10^{-7}$</td>
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<tr>
<td>Benzo(a)pyrene</td>
<td>191-24-2</td>
<td>276.34</td>
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<td>$1.3 \times 10^{-7}$</td>
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<td>Benzo(g,h,i)perylene</td>
<td>193-39-5</td>
<td>276.34</td>
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<td>Indeno(1,2,3-cd)pyrene</td>
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**Polychlorinated biphenyls**

*(Indicator-PCBs)** *(PCB7)*

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<td>35693-99-3</td>
<td>291.99</td>
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<td>PCB 101</td>
<td>37680-73-2</td>
<td>236.44</td>
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<td>PCB 118*</td>
<td>31508-00-6</td>
<td>326.44</td>
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<tr>
<td>PCB 138</td>
<td>35065-28-2</td>
<td>360.88</td>
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<tr>
<td>PCB 153</td>
<td>35065-27-1</td>
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<tr>
<td>PCB 180</td>
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<td>395.33</td>
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**Polybrominated diphenylethers (PBDEs)**

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<th>41318-75-6</th>
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<td>PBDE 99**</td>
<td>60348-60-9</td>
<td>564.69</td>
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<td>1.2 $\times 10^{-6}$</td>
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<td>PBDE 100**</td>
<td>189084-64-8</td>
<td>564.69</td>
<td>7.66</td>
<td>1.1 $\times 10^{-2}$</td>
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<tr>
<td>PBDE 153**</td>
<td>68631-49-2</td>
<td>643.59</td>
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<td>PBDE 154**</td>
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<tr>
<td>PBDE 183**</td>
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<td>722.48</td>
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<tr>
<td>PBDE 209</td>
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<td>959.17</td>
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**Polychlorinated alkanes (PCAs)**

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<th>85535-84-8</th>
<th>Physicochemical properties depend on the degree of chlorination</th>
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<td>SCCP*</td>
<td>85535-85-9</td>
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<td>MCCP</td>
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**Siloxanes (not included in the PCA model)**

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<th>556-67-2</th>
<th>296.62</th>
<th>5.09</th>
<th>0.17</th>
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<tbody>
<tr>
<td>Octamethylcyclotetrasiloxane</td>
<td>541-02-6</td>
<td>370.78</td>
<td>5.71</td>
<td>1.9 $\times 10^{-2}$</td>
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<td>Decamethylcyclopentasiloxane</td>
<td>540-97-6</td>
<td>444.93</td>
<td>6.33</td>
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<td>Dodecamethylcyclohexasiloxane</td>
<td>107-46-0</td>
<td>162.39</td>
<td>4.76</td>
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<td>Hexamethyldisiloxane</td>
<td>107-51-7</td>
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<td>Octamethyltrisiloxane</td>
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<td>Decamethyldisiloxane</td>
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**Terpenes (not included in the PCA model)**

<table>
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<th>136.24</th>
<th>4.83</th>
<th>44</th>
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<tbody>
<tr>
<td>D-limonene</td>
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<td>136.24</td>
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### Fluorinated compounds

**Perfluorochemicals (PFCs)**

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<th>LogKoc</th>
<th>LogKow</th>
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<td>Perfluorohexane (PFHxS)</td>
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<td>Perfluorotridecane (PFTrDA)</td>
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**Organometals**

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<td>Dibutyltin (DBT)</td>
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<td>Tributyltin* (TBT)</td>
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**Metals**

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<td>Zn</td>
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**Insecticides**

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**Herbicides**

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**Fungicides**

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*Fungicides*
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<th>Molecular weight.</th>
<th>octanol-water partition coefficient, estimated values.</th>
<th>Water Solubility.</th>
<th>The commercial mixture contains four isomers, of which tris(2-chloroisopropyl) phosphate is the most abundant.</th>
<th>Experimental value (Takacs-Novak et al., 1992).</th>
<th>PCB 118 is classified both as WHO- and Indicator-PCB.</th>
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Table S2  Comparative data of the analytical techniques and quantifying uncertainties in the analyses of the compounds

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<th>Analytical technique</th>
<th>Quantifying uncertainty (%)</th>
<th>Reference</th>
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<td>GC-MS</td>
<td>± 40</td>
<td>(IVL, 2006a)</td>
</tr>
<tr>
<td></td>
<td>Hormones</td>
<td>LC-TOF-MS</td>
<td>± 40</td>
<td>(IVL, 2006a)</td>
</tr>
<tr>
<td>Dioxin-like compounds</td>
<td>WHO-PCBs</td>
<td>GC-HRMS</td>
<td>± 29</td>
<td>(Liljelind et al., 2003)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>PCDD/Fs</td>
<td>GC-HRMS</td>
<td>± 29</td>
<td>(Liljelind et al., 2003)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Other POPs</td>
<td>Polycyclic aromatic hydrocarbons</td>
<td>GC-MS</td>
<td>± 30</td>
<td>(Swedish EPA, 1990)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Indicator-PCBs</td>
<td>GC-MS</td>
<td>± 30</td>
<td>(Swedish EPA, 1990)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Polybrominated diphenylethers</td>
<td>GC-MS</td>
<td>± 30</td>
<td>(Liljelind et al., 2003)&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Chloroparaffins</td>
<td>GC-MS</td>
<td>± 30</td>
<td>(Reth et al., 2005)&lt;sup&gt;d,f&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Siloxanes</td>
<td>ATD-GC-MS</td>
<td>± 40</td>
<td>(IVL, 2005b)</td>
</tr>
<tr>
<td></td>
<td>Terpene (Limonene)</td>
<td>ATD-GC-FID</td>
<td>± 40</td>
<td>(IVL, 2005c)</td>
</tr>
<tr>
<td>Fluorinated compounds</td>
<td>Perfluorocarbons</td>
<td>LC-MS/MS</td>
<td>± 5-20</td>
<td>(Karrman et al., 2005)&lt;sup&gt;g&lt;/sup&gt;</td>
</tr>
<tr>
<td>Organometals</td>
<td>Organotin compounds</td>
<td>ICP-MS</td>
<td>± 6-40</td>
<td>(Kumar et al., 2003)&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td>Metals</td>
<td>As, Cd, Co, Cr, Hg, Ni, Pb</td>
<td>ICP- SFMS</td>
<td>± 20</td>
<td>(U.S.EPA, 1994a)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Cu, V, Zn</td>
<td>ICP- AES</td>
<td>± 20-30</td>
<td>(U.S.EPA, 1994b)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Pesticides</td>
<td>Insecticides, herbicides, and fungicides</td>
<td>GC-MS</td>
<td>± 40</td>
<td>CL&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td>Biocides</td>
<td></td>
<td>GC-MS</td>
<td>± 40</td>
<td>(IVL, 2006b)</td>
</tr>
</tbody>
</table>

<sup>a</sup>GC, Gas Chromatography; MS, Mass Spectrometry; LC, Liquid Chromatography; MS/MS, Tandem Mass Spectrometry; TOF, Time-of-Flight; HRMS, High Resolution Mass Spectrometry; ATD, Automated Thermal Desorption; FID, Flame Ionization Detection; ICP, Inductively Coupled Plasma; SFMS, Sector Field Mass Spectrometry; and AES, Atomic Emission Spectrometry. <sup>b</sup>CL, Commercial Laboratory. <sup>c</sup>Accredited analysis. <sup>d</sup>In-house validated analytical method. <sup>e</sup>BHT semi-quantitatively analyzed, the results are presented in benzylbenzoate-equivalents. <sup>f</sup>Modification: <sup>13</sup>C labelled PCB 188 was used as recovery standard instead of ε-HCH. <sup>g</sup>With some modifications.
*priority substance included in the WFD (EU, 2000), **classified as POP according to the Stockholm Convention (UNEP, 2001), abbreviations of the compounds used in the PCA model are presented in parenthesis

<table>
<thead>
<tr>
<th>Chemical</th>
<th>STP A</th>
<th>STP B</th>
<th>STP C</th>
<th>STP D</th>
<th>STP E</th>
<th>STP F</th>
<th>STP G</th>
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<tbody>
<tr>
<td><strong>Chlorophenols (CPs)</strong></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>2-monochlorophenol (2-CP)</td>
<td>0.022</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>0.028</td>
<td>0.036</td>
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<tr>
<td>3-monochlorophenol (3-CP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>4-monochlorophenol (4-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<tr>
<td>2,3-dichlorophenol (23-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>0.028</td>
<td>0.036</td>
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<tr>
<td>2,4-dichlorophenol (24-CP)+</td>
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<td>0.07</td>
<td>0.034</td>
<td>&lt;0.02</td>
<td>0.062</td>
<td>0.021</td>
<td>0.064</td>
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<tr>
<td>2,6-dichlorophenol (26-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<td>&lt;0.02</td>
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<tr>
<td>3,4-dichlorophenol (34-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<tr>
<td>3,5-dichlorophenol (35-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<tr>
<td>2,3,4-trichlorophenol (234-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<tr>
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<td>&lt;0.02</td>
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<td>&lt;0.02</td>
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<tr>
<td>2,3,6-trichlorophenol (236-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>2,4,5-trichlorophenol (245-CP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>2,4,6-trichlorophenol (246-CP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>3,4,5-trichlorophenol (345-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>2,3,4,5-tetrachlorophenol (2345-CP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>2,3,4,6-tetrachlorophenol (2346-CP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>2,3,5,6-tetrachlorophenol (2356-CP)</td>
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<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td>Pentachlorophenol* (PCP)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
</tr>
<tr>
<td><strong>4-Nonylphenol</strong> (4NP)</td>
<td>20</td>
<td>21</td>
<td>8</td>
<td>12</td>
<td>40</td>
<td>13.1</td>
<td>10</td>
</tr>
<tr>
<td>Butylhydroxytoluene (BHT)</td>
<td>0.81</td>
<td>0.64</td>
<td>0.83</td>
<td>1.5</td>
<td>2.4</td>
<td>1.6</td>
<td>2.2</td>
</tr>
<tr>
<td>Triclosan (TCS)</td>
<td>4.6</td>
<td>8.3</td>
<td>1.8</td>
<td>5.5</td>
<td>3.7</td>
<td>2.4</td>
<td>3.4</td>
</tr>
</tbody>
</table>

| **Chlorobenzenes**         |        |        |        |        |        |        |        |
| 1,2-dichlorobenzene (12CBz)| 7       | 3      | <0.003 | <0.003 | 79     | 2      | <0.003 |
| 1,3-dichlorobenzene (13CBz)+| 26     | 5      | <0.003 | 14     | 64     | 29     | 8      |
| 1,4-dichlorobenzene (14CBz)| <0.003 | <0.003 | 149    | <0.003 | <0.003 | <0.003 | <0.003 |
| 1,2,3-trichlorobenzene* (123CBz)| <0.003 | <0.003 | 541    | <0.003 | <0.003 | <0.003 | <0.003 |
| 1,2,4-trichlorobenzene* (124CBz)| <0.003 | <0.003 | <0.003 | 541    | <0.003 | <0.003 | <0.003 |
| 1,3,5-trichlorobenzene* (135CBz)| <0.003 | <0.003 | <0.003 | <0.003 | <0.003 | <0.003 | <0.003 |
| 1,2,3,4-tetrachlorobenzene (1234CBz)| <0.002 | <0.002 | 4      | <0.002 | <0.002 | <0.002 | <0.002 |
| 1,2,3,5-tetrachlorobenzene (1235CBz)+| 0.9    | 1      | 5      | 1      | 4      | 1      | 1      |
| 1,2,4,5-tetrachlorobenzene (1245CBz)| 0.4    | 0.5    | 1      | 1      | 3      | 1      | 1      |
| Pentachlorobenzene* ** (PCBz)| 0.4    | 0.5    | 1      | 1      | 3      | 1      | 1      |
| Hexachlorobenzene* ** (HCBz)| 4      | 9      | 6      | 9      | 20     | 6      | 4      |
### Esters

<table>
<thead>
<tr>
<th>Organophosphorus compounds (OPs)</th>
<th>µg kg⁻¹ d.w.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tributyl phosphate (TBP)</td>
<td>7 11 37 24 10 37 14</td>
</tr>
<tr>
<td>Tris(2-chloroethyl) phosphite (TCP)</td>
<td>3 5 9 8 4 20 &lt;2</td>
</tr>
<tr>
<td>Tris(2-chloroisopropyl) phosphite (TCP)</td>
<td>559 409 916 859 547 1545 209</td>
</tr>
<tr>
<td>Tris(1,3-dichloro-2-propyl) phosphite (TDCPP)</td>
<td>24 55 22 40 32 309 56</td>
</tr>
<tr>
<td>Tris(2-butoxyethyl) phosphate (TBP)</td>
<td>94 210 &lt;32 1865 &lt;32 &lt;32 &lt;32</td>
</tr>
</tbody>
</table>

### Phthalates

<table>
<thead>
<tr>
<th>Phthalate</th>
<th>µg kg⁻¹ d.w.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimethyl phthalate (DMP)</td>
<td>&lt;0.75 &lt;0.70 &lt;0.11 &lt;3.2 &lt;0.10 &lt;0.47 &lt;0.68</td>
</tr>
<tr>
<td>Diethyl phthalate (DEP)</td>
<td>&lt;0.075 &lt;0.07 &lt;0.11 &lt;0.065 &lt;0.10 &lt;0.047 &lt;0.068</td>
</tr>
<tr>
<td>Di-n-butyl phthalate (DBP)</td>
<td>&lt;0.075 &lt;0.70 &lt;0.11 &lt;3.2 &lt;0.10 &lt;0.47 &lt;0.68</td>
</tr>
<tr>
<td>Butylbenzyl phthalate (BBP)</td>
<td>&lt;0.075 &lt;0.07 &lt;0.11 &lt;0.065 &lt;0.10 &lt;0.047 &lt;0.068</td>
</tr>
<tr>
<td>Di-(2-ethylhexyl) phthalate (DEHP)*</td>
<td>60 95 34 220 41 60 65</td>
</tr>
<tr>
<td>Di-n-octyl phthalate (DNOP)</td>
<td>&lt;0.075 &lt;0.07 &lt;0.11 &lt;0.065 &lt;0.10 &lt;0.047 &lt;0.068</td>
</tr>
<tr>
<td>Di-&lt;i&gt;iso&lt;/i&gt;-decyl phthalate (DIDP)</td>
<td>30 35 14 23 54 21 10</td>
</tr>
<tr>
<td>Di-&lt;i&gt;iso&lt;/i&gt;-nonyl phthalate (DINP)</td>
<td>32 60 21 78 24 31 29</td>
</tr>
</tbody>
</table>

### Phthalates (not included in the PCA model)

<table>
<thead>
<tr>
<th>Adipate</th>
<th>µg kg⁻¹ d.w.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diethyl adipate</td>
<td>&lt;5 n.m. n.m. n.m. n.m. n.m. &lt;5</td>
</tr>
<tr>
<td>Di-&lt;i&gt;iso&lt;/i&gt;-butyl adipate</td>
<td>&lt;10 n.m. n.m. n.m. n.m. n.m. &lt;10</td>
</tr>
<tr>
<td>Dibutyl adipate</td>
<td>&lt;10 n.m. n.m. n.m. n.m. n.m. &lt;10</td>
</tr>
<tr>
<td>Di-(2-ethylhexyl) adipate</td>
<td>100 n.m. n.m. n.m. n.m. n.m. 40</td>
</tr>
<tr>
<td>Dioctyl adipate</td>
<td>&lt;5 n.m. n.m. n.m. n.m. n.m. &lt;5</td>
</tr>
<tr>
<td>Didecyl adipate</td>
<td>&lt;10 n.m. n.m. n.m. n.m. n.m. &lt;10</td>
</tr>
<tr>
<td>Di-&lt;i&gt;iso&lt;/i&gt;-octyl adipate</td>
<td>&lt;50 n.m. n.m. n.m. n.m. n.m. &lt;50</td>
</tr>
<tr>
<td>Di-&lt;i&gt;iso&lt;/i&gt;-decyl adipate</td>
<td>&lt;50 n.m. n.m. n.m. n.m. n.m. &lt;50</td>
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### Antibiotics

<table>
<thead>
<tr>
<th>Fluoroquinolones (FQs)</th>
<th>mg kg⁻¹ d.w.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Norfloxacin (Nor)</td>
<td>5.3 4.2 3.9 4.2 5.0 5.5 3.0</td>
</tr>
<tr>
<td>Ofloxacin (OfI)</td>
<td>1.3 1.3 &lt;0.1 1.2 1.7 1.7 &lt;0.1</td>
</tr>
<tr>
<td>Ciprofloxacin (Cip)</td>
<td>8.2 7.6 6.0 7.9 9.3 8.8 3.9</td>
</tr>
</tbody>
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### Tetracyclines (not included in the PCA model)

<table>
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<th>Tetracycline</th>
<th>µg kg⁻¹ d.w.</th>
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<tbody>
<tr>
<td>Oxytetracycline</td>
<td>&lt;4 n.m. 1400 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Tetracycline</td>
<td>3000 n.m. &lt;3 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Demeclocycline</td>
<td>&lt;4 n.m. &lt;6 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Chlorotetracycline</td>
<td>&lt;8 n.m. &lt;12 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Doxycycline</td>
<td>1100 n.m. &lt;6 n.m. n.m. n.m. n.m.</td>
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### Pharmaceuticals (not included in the PCA model)

<table>
<thead>
<tr>
<th>Non-steroid anti-inflammatory drugs (NSAIDs)</th>
<th>µg kg⁻¹ d.w.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ibuprofen</td>
<td>130 n.m. 33 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Naproxen</td>
<td>7.6 n.m. &lt;4 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Ketoprofen</td>
<td>12 n.m. &lt;9 n.m. n.m. n.m. n.m.</td>
</tr>
<tr>
<td>Diclofenac</td>
<td>77 n.m. 16 n.m. n.m. n.m. n.m.</td>
</tr>
</tbody>
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### Hormones

<table>
<thead>
<tr>
<th></th>
<th>µg kg⁻¹ d.w.</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Estriol</td>
<td>&lt;1</td>
<td>n.m.</td>
<td>&lt;2</td>
<td>n.m.</td>
<td>n.m.</td>
<td>n.m.</td>
</tr>
<tr>
<td>Estradiol</td>
<td>&lt;2</td>
<td>n.m.</td>
<td>&lt;2</td>
<td>n.m.</td>
<td>n.m.</td>
<td>n.m.</td>
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<tr>
<td>Ethinylestradiol</td>
<td>&lt;3</td>
<td>n.m.</td>
<td>&lt;4</td>
<td>n.m.</td>
<td>n.m.</td>
<td>n.m.</td>
</tr>
<tr>
<td>Norethindrone</td>
<td>&lt;6</td>
<td>n.m.</td>
<td>&lt;9</td>
<td>n.m.</td>
<td>n.m.</td>
<td>n.m.</td>
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### Polychlorinated biphenyls (WHO-PCBs)**

<table>
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<tr>
<th></th>
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<tr>
<td>PCB 77</td>
<td>167</td>
<td>97</td>
<td>99</td>
<td>99</td>
<td>140</td>
<td>89</td>
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<td>PCB 81</td>
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<td>&lt;0.3</td>
<td>&lt;0.3</td>
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<td>PCB 126</td>
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<td>PCB 169</td>
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<td>3</td>
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<td>PCB 105</td>
<td>2314</td>
<td>1161</td>
<td>841</td>
<td>1487</td>
<td>2436</td>
<td>2774</td>
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<tr>
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### Dioxin-like compounds

#### Polychlorinated dibenzo-β-oxins and -furans (PCDD/Fs)**

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<td>&lt;3</td>
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<td>1,2,3,4,6,7,8-HпCDF (1234678-CDF)</td>
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<td>260</td>
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<td>222</td>
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S16
### Other organic compounds

#### Polycyclic aromatic hydrocarbons (PAHs)*

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<th>Concentration (mg kg⁻¹ d.w.)</th>
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<td>Fluoranthene</td>
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<tr>
<td>Benzo(b)fluoranthene</td>
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<td>Benzo(k)fluoranthene</td>
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<td>Benzo(a)pyrene</td>
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<tr>
<td>Benzo(g,h,i)perylene</td>
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<tr>
<td>Indeno(1,2,3-cd)pyrene</td>
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#### Polychlorinated biphenyls (Indicator-PCBs)***

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<th>Concentration (mg kg⁻¹ d.w.)</th>
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<tr>
<td>PCB 52</td>
<td>0.006</td>
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<tr>
<td>PCB 101</td>
<td>0.009</td>
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<tr>
<td>PCB 118*</td>
<td>0.006</td>
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<tr>
<td>PCB 138</td>
<td>0.019</td>
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<tr>
<td>PCB 153</td>
<td>0.017</td>
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<tr>
<td>PCB 180</td>
<td>0.009</td>
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#### Polybrominated diphenylethers (PBDEs)

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<tr>
<td>PBDE 28*</td>
<td>0.26</td>
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<td>PBDE 47* - **</td>
<td>&lt;0.9</td>
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<tr>
<td>PBDE 99* - **</td>
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<tr>
<td>PBDE 100* - **</td>
<td>&lt;0.7</td>
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<tr>
<td>PBDE 153* - **</td>
<td>&lt;0.7</td>
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<tr>
<td>PBDE 154* - **</td>
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<td>PBDE 183*</td>
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#### Polychlorinated alkanes (PCAs)

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<tr>
<td>MCCP</td>
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<td>LCCP</td>
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#### Siloxanes (not included in the PCA model)

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<tr>
<td>Octamethylcyclotetrasiloxane</td>
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<td>Decamethylcyclopentasiloxane</td>
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<td>Dodecamethylcyclohexasiloxane</td>
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<tr>
<td>Hexamethyldisiloxane</td>
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<tr>
<td>Octamethyltrisiloxane</td>
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<tr>
<td>Decamethyltetrasiloxane</td>
<td>16</td>
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<td>Dodecamethyltetrasiloxane</td>
<td>46</td>
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#### Terpenes (not included in the PCA model)

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<th>Concentration (µg kg⁻¹ d.w.)</th>
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<tbody>
<tr>
<td>D-limonene</td>
<td>150</td>
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<tr>
<td>L-limonene</td>
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## Fluorinated compounds

### Perfluorochemicals (PFCs)  \( \mu g \, kg^{-1} \, d.w. \)

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<th>3.0</th>
<th>5.4</th>
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<tr>
<td>Perfluorohexane acid (PFHxA)</td>
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<tr>
<td>Perfluoroheptane acid (PFHpA)</td>
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<td>&lt;0.5</td>
<td>&lt;0.5</td>
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<td>Perfluorooctane acid (PFOS)</td>
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<td>1.3</td>
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<td>Perfluorooctonane acid (PFNOA)</td>
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<td>&lt;0.4</td>
<td>&lt;0.4</td>
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<td>Perfluorodecane acid (PFDA)</td>
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<td>&lt;0.8</td>
<td>&lt;0.8</td>
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<td>Perfluoroundecane acid (PFUnA)</td>
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<td>&lt;1.5</td>
<td>&lt;1.5</td>
<td>&lt;1.5</td>
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<td>Perfluorohexane sulfonate (PFHxS)</td>
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<tr>
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## Organometals

### Organotin compounds (OTCs)  \( \mu g \, kg^{-1} \, d.w. \)

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## Metals  \( mg \, kg^{-1} \, d.w. \)

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<th>Cu</th>
<th>Hg</th>
<th>Ni</th>
<th>Pb</th>
<th>V</th>
<th>Zn</th>
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## Insecticides  \( \mu g \, g^{-1} \, d.w. \)

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<th>n.q.</th>
<th>n.q.</th>
<th>n.q.</th>
<th>n.q.</th>
<th>n.q.</th>
<th>n.q.</th>
<th>n.q.</th>
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<tbody>
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<td>&lt;0.006</td>
<td>&lt;0.006</td>
<td>&lt;0.006</td>
<td>&lt;0.006</td>
<td>&lt;0.006</td>
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<td>&lt;0.006</td>
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<td>Terbutylazine desethyl*</td>
<td>n.q. n.q. n.q. n.q. n.q. n.q. n.q. n.q.</td>
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<tr>
<td>Terbutryn</td>
<td>n.q.</td>
</tr>
<tr>
<td>Terbutylazine</td>
<td>&lt;0.1 &lt;0.1 &lt;0.1 &lt;0.1 &lt;0.1 &lt;0.1 &lt;0.1 &lt;0.1</td>
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<tr>
<td>Trifluralin*</td>
<td>&lt;0.005 &lt;0.005 &lt;0.005 &lt;0.005 &lt;0.005 &lt;0.005 &lt;0.005 &lt;0.005</td>
</tr>
</tbody>
</table>
Biocides

<table>
<thead>
<tr>
<th>Compound</th>
<th>µg kg⁻¹ d.w.</th>
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</thead>
<tbody>
<tr>
<td>2-Mercaptobenzothiazole (2MERCAPTOB)</td>
<td>&lt;25 200 &lt;20 250 280 22 950</td>
</tr>
<tr>
<td>2-(Tiocyanomethylthio)benzothiazole (2TIOCYANOM)</td>
<td>&lt;50 &lt;50 &lt;50 &lt;50 &lt;50 &lt;50 &lt;50</td>
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<tr>
<td>4-Chloro-3-cresol (KLORKRESOL)</td>
<td>30 19 59 6.8 67 14 &lt;3</td>
</tr>
<tr>
<td>N-didecyldimethylammonium chloride (DDMAC)</td>
<td>13000 14000 5600 1400 61000 21000 3000</td>
</tr>
<tr>
<td>Propiconazole (PROPICONA)</td>
<td>&lt;2 &lt;5 &lt;5 &lt;0.01 &lt;5 &lt;5 &lt;5</td>
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<tr>
<td>Resorcinol (RESORCINOL)</td>
<td>&lt;10 &lt;25 &lt;50 &lt;10 160 &lt;20 50</td>
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<tr>
<td>Methylparabene (MEPARAB)</td>
<td>15 52 13 44 59 29 18</td>
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<tr>
<td>Ethylparabene (ETPARAB)</td>
<td>&lt;10 &lt;4 &lt;7 &lt;4 &lt;30 &lt;5 &lt;3</td>
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<tr>
<td>Propylparabene (PROPARAB)</td>
<td>&lt;4 &lt;4 &lt;7 &lt;4 &lt;23 &lt;6 3.6</td>
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<tr>
<td>Butylparabene (BUPARAB)</td>
<td>&lt;4 &lt;4 &lt;7 &lt;4 &lt;23 &lt;5 &lt;3</td>
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<tr>
<td>Benzylparabene (BEPARAB)</td>
<td>&lt;6 &lt;7 &lt;12 &lt;6 &lt;36 &lt;8 &lt;5</td>
</tr>
</tbody>
</table>

n.m., not measured. n.q., not quantifiable. n.d., not detected.

References


