Comprehensive mass flow analysis of Swedish sludge contaminants

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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⁻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-*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.

Keywords: PPCP, POP, sewage sludge, emerging pollutants.

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 $\frac{1}{2}LoD$. 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; Σ PAH₉, 6; and Σ PCB₇, 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 $<1 \text{ mg kg}^{-1} \text{ d.w.}$; 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 $<10^{-5} \text{ atm m}^3 \text{ mol}^{-1}$) 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 $>5 \text{ mg L}^{-1}$; 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 (Petersson, 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.

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

Compounds	n ^a	Applications	Quantity (10 ³ kg year ⁻¹) ^b
As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn	10	Metals	21 046
Phthalates	8	Softening agent in plastics	73 964
Biocides	11	Killing living organisms	1 637
Polycyclic aromatic hydrocarbons (PAHs)	6	Products of incomplete combustion	1 203 ^c
Adipates	8	Softening agent in plastics	1 073
Pesticides	109	Control pests	828
Polychlorinated alkanes (PCAs)	3	Lubricants and cutting fluids (metal working industry), and plasticizers	298
Organophosphorus compounds (OPs)	6	Flame retardants and/or plasticizers in textiles, plastics, and building materials	286
Butylhydroxytoluene (BHT)	1	Stabilizer in plastics and rubber, antioxidant (ex. processed food)	254
Organotin compounds (OTCs)	6	In anti-fouling compositions and stabilizer in polyvinyl chloride (PVC)	240
Non-steroid anti-inflammatory drugs (NSAIDs)	4	Pharmaceuticals	84 ^d
Siloxanes	7	Sanitary articles, lubricants and hydraulic fluids in textiles and skin care products	31
Perfluorochemicals (PFCs)	13	Water, fat or stain repellents for paper, textiles, carpets, etc.	24 ^e
Terpene (Limonene)	2	Flavor and odor additive (hygiene products and perfumes)	17
Polychlorobenzenes (PCBz)	11	Dyestuffs and solvent for pesticides	8.1 ^f
4-Nonylphenol	1	Detergent, surfactants (metabolite)	7.6
Fluoroquinolones (FQs)	3	Pharmaceuticals (antibiotics)	5.1 ^g
Polybrominated diphenylethers (PBDEs)	8	Flame retardants in electronics, furniture, and building materials	3.6 ^h
Triclosan	1	Antibacterial in toothpaste and deodorants (personal care products)	3.1
Tetracyclines (TCs)	5	Pharmaceuticals (antibiotics)	1.3 ^{d,i}
Hormones	4	Pharmaceuticals	0.07 ^d
Chlorophenols (CPs)	19	Wood and textile preservatives	Banned (1978) ^j
Polychlorinated biphenyls (PCBs)		Dielectric fluids in transformers and capacitors	Banned (1972) ^j
WHO-PCBs	12		
Indicator-PCBs (I-PCBs)	7		
Polychlorinated dibenzo- <i>p</i> -dioxins and furans (PCDD/Fs)	17	Unintentionally formed (by-products)	-

^an: number of compounds included in the group. ^bAnnual quantity, in Sweden 2004, recorded in the products and pesticides register (Swedish Chemicals Agency, 2007b). ^cQuantity of benzo(a)pyrene. ^dThe Swedish Medical Products Agency (MPA). ^eSwedish Chemical Agency (2006). ^fQuantity of 1,2-dichlorobenzene. ^gLindberg et al. (2005). ^hQuantity of PBDE 209. ⁱdemeclocycline and chlorotetracycline not included. ^jIn Sweden.

Table 2 Physicochemical properties of the studied compounds (EPI Suite™, 2007)

Class of compound	Sub group	M _w (g mol ⁻¹) ^a	log K _{ow} ^b	S _w (mg L ⁻¹) ^c	H (atm·m ³ mol ⁻¹) ^d
Metals	As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn	51 - 207	-0.6 - 0.7	6·10 ⁴ - 4·10 ⁵	2·10 ⁻² - 0.8
Esters	Phthalates	194 - 447	1.7 - 10	1·10 ⁻⁵ - 8·10 ³	4·10 ⁻⁸ - 4·10 ⁻⁵
	Adipates	202 - 427	2.4 - 10	4·10 ⁻⁶ - 690	2·10 ⁻⁶ - 2·10 ⁻⁴
	OPs	266 - 431	1.6 - 4.7	5 - 6·10 ³	1·10 ⁻¹¹ - 3·10 ⁻⁶
Pesticides	Biocides	110 - 362	1 - 4.7	7·10 ⁻⁶ - 3·10 ⁵	6·10 ⁻¹² - 5·10 ⁻⁷
	Insecticides	183 - 505	-0.9 - 7.4	2·10 ⁻³ - 1·10 ⁶	3·10 ⁻¹² - 4·10 ⁻⁴
	Herbicides	111 - 412	-4.5 - 5.3	5·10 ⁻² - 1·10 ⁶	4·10 ⁻¹⁹ - 2·10 ⁻⁴
	Fungicides	169 - 403	0.9 - 5.5	4·10 ⁻² - 9·10 ³	8·10 ⁻¹⁴ - 3·10 ⁻⁵
Hydrocarbons	PAHs	202 - 276	4.9 - 6.7	2·10 ⁻⁴ - 9·10 ⁻²	1·10 ⁻⁷ - 8·10 ⁻⁶
	Terpene (Limonene)	136	4.8	44	0.4
Phenols	Chlorophenols	129 - 266	2.2 - 4.7	45 - 1·10 ⁴	1·10 ⁻⁷ - 4·10 ⁻⁷
	Butylhydroxytoluene	220	5.0	10	4·10 ⁻⁶
	Triclosan	290	4.7	9.3	5·10 ⁻⁹
	4-Nonylphenol	220	5.9	2.7	6·10 ⁻⁶
Organometals	Organotin compounds	177 - 351	0.6 - 7.4	6·10 ⁻⁷ - 4·10 ³	1·10 ⁻⁹ - 1.5
Pharmaceuticals	Fluoroquinolones	319 - 361	-0.3 - 0.3 ^e	7·10 ³ - 4·10 ⁴	5·10 ⁻²⁰ - 9·10 ⁻¹⁹
	Tetracyclines	444 - 483	-4 - -0.7	160 - 3·10 ⁵	1·10 ⁻³¹ - 5·10 ⁻²⁴
	NSAIDs	206 - 296	3.0 - 4.0	11 - 260	5·10 ⁻¹² - 2·10 ⁻⁷
	Hormones	272 - 298	2.8 - 4.1	13 - 560	1·10 ⁻¹² - 6·10 ⁻¹⁰
Siloxanes	Methylsiloxanes	162 - 445	4.8 - 6.5	1·10 ⁻⁴ - 1.4	9·10 ⁻² - 0.8
Fluorinated compounds	Perfluorochemicals	314 - 714	2.2 - 12	6·10 ⁻⁷ - 2	1·10 ⁻⁹ - 2·10 ³
Halogenated compounds	Polychlorobenzenes	147 - 285	3.3 - 5.9	0.3 - 100	9·10 ⁻⁴ - 3·10 ⁻³
	PBDEs	407 - 959	5.9 - 12	3·10 ⁻⁶ - 0.3	1·10 ⁻⁸ - 7·10 ⁻⁶
	I-PCBs	258 - 395	5.7 - 8.3	4·10 ⁻⁴ - 0.1	5·10 ⁻⁵ - 2·10 ⁻⁴
	WHO-PCBs	292 - 395	6.3 - 8.3	4·10 ⁻⁴ - 3·10 ⁻²	5·10 ⁻⁵ - 1·10 ⁻⁴
	PCDD/Fs	306 - 460	6.3 - 9.5	9·10 ⁻⁶ - 3·10 ⁻²	1·10 ⁻⁶ - 2·10 ⁻⁵
	PCAs		Depend on the degree of chlorination		

Abbreviations can be found in Table 1. ^aM_w: Molecular weight. ^blog K_{ow}: octanol-water partition coefficient, estimated values. ^cS_w: Water solubility, estimated values. ^dH: Henry's Law Constant, estimated values. ^eExperimentally determined value (Takacs-Novak et al., 1992).

Table 3 Descriptive data of the investigated sewage treatment plants (STPs) (STPs, 2005)

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

^aInd., industry; mix, mixture of industrial sewage; F, food; H, hospital; T, textile; C, chemical; L, laundry; and House, household. ^bM, mechanical; C, chemical; B, biological treatment (activated sludge); D, digestion (anaerobic); and S, stabilization (aerobic) of the sludge. ^cSolid retention time in the digester/aerobic stabilizer. ^dPercentage of the total annual production of sewage sludge in Sweden (Swedish EPA, 2007).

^ePercent 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

Compounds	Det. Freq. ^a	Measured concentrations (MC) ($\mu\text{g kg}^{-1}$ d.w.)				MF (kg year^{-1}) ^c	Rec. (%) ^d
		min	max	average	RSD (%) ^b		
As, Cd, Co, Cr, Cu, Hg, Ni, Pb, V, Zn	7/7	500 000	1 100 000	800 000	23	190 000	0.91
Phthalates	7/7	69 000	320 000	120 000	57	29 000	0.04
Polychlorinated alkanes (PCAs)	7/7	9 900	82 000	50 000	56	12 000	4.1
Siloxanes	3/3	13 000	25 000	22 000	33	5 300	17
Biocides	7/7	4 000	62 000	14 000	102	3 400	0.21
4-Nonylphenol	7/7	8 000	40 000	13 000	26	3 100	41
Fluoroquinolones (FQs)	7/7	7 000	16 000	13 000	62	3 200	63
Triclosan	7/7	1 800	8 300	3 700	51	890	29
Tetracyclines (TCs)	2/2	1 400	4 100	2 800	70	660	51
Pesticides	4/7	2 100	10 000	2 100	115	500	0.06
Butylhydroxytoluene (BHT)	7/7	640	2 400	1 500	49	360	0.14
Organophosphorus compounds (OPs)	7/7	310	2 800	730	78	170	0.06
Polycyclic aromatic hydrocarbons (PAHs)	6/7	470	1 700	640	76	150	0.01
Polybrominated diphenylethers (PBDEs)	7/7	390	870	550	28	130	3.7
Organotin compounds (OTCs)	7/7	230	480	410	29	99	0.04
Terpene (Limonene)	2/2	150	500	330	75	78	0.46
Non-steroid anti-inflammatory drugs (NSAIDs)	2/2	62	230	140	81	35	0.04
Chlorophenols (CPs)	6/7	34	130	92	61	22	–
Adipates	2/2	40	100	70	61	17	0.002
Indicator-PCBs	7/7	23	100	50	67	12	–
Polychlorobenzenes	7/7	20	330	39	126	9.3	0.11
Perfluorochemicals (PFCs)	7/7	13	290	38	128	9.2	0.04
WHO-PCBs	7/7	3.2	11	6	44	1.4	–
Polychlorinated dioxins/furans (PCDD/Fs)	7/7	0.96	2.2	1.6	25	0.4	–
Hormones	0/2	<LoD ^e	<LoD	<LoD	–	–	–

^aNumber of positive samples/number of STPs. ^bRSD: Relative Standard Deviation. ^cMF: Mass Flow, based on MC and the annual production of sewage sludge (Swedish EPA, 2007). ^dPercentage of the compounds recovered in sewage sludge, of the annual quantity recorded in Sweden in 2004 (Swedish Chemicals Agency, 2007b). ^eLoD: 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, PFOA, PFDA, PFUnA, PFNA, PFTrDA, 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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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, perfluorooctane acid; PFNA, perfluorononane acid; PFOS, perfluorooctane sulfonate; PFOSA, perfluorooctane sulfonamide; PFDA, perfluorodecane acid; PFUnA, perfluoroundecane acid; PFDS, perfluorodecane sulfonate; PFDoA, perfluorododecane acid; PFTeDA, perfluorotetradecane acid and PFTeDA, perfluorotetradecane 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

Chemical	CAS RN ^a	M _w (g mol ⁻¹) ^b	log K _{ow} ^c	S _w (mg L ⁻¹) ^d	Henry's Law Constant ^e
Phenols					
Chlorophenols (CPs)					
2-monochlorophenol (2-CP)	95-57-8	128.56	2.16	12 734	4.2·10 ⁻⁷
3-monochlorophenol (3-CP)	108-43-0	128.56	2.16	12 734	4.2·10 ⁻⁷
4-monochlorophenol (4-CP)	106-48-9	128.56	2.16	12 734	4.2·10 ⁻⁷
2,3-dichlorophenol (23-CP)	576-24-9	163.00	2.80	3 282	3.1·10 ⁻⁷
2,4-dichlorophenol (24-CP)	120-83-2	163.00	2.80	3 282	3.1·10 ⁻⁷
2,5-dichlorophenol (25-CP)	583-78-8	163.00	2.80	3 282	3.1·10 ⁻⁷
2,6-dichlorophenol (26-CP)	87-65-0	163.00	2.80	3 282	3.1·10 ⁻⁷
3,4-dichlorophenol (34-CP)	95-77-2	163.00	2.80	3 282	3.1·10 ⁻⁷
3,5-dichlorophenol (35-CP)	591-35-5	163.00	2.80	3 282	3.1·10 ⁻⁷
2,3,4-trichlorophenol (234-CP)	15950-66-0	197.45	3.45	808	2.3·10 ⁻⁷
2,3,5-trichlorophenol (235-CP)	933-78-8	197.45	3.45	808	2.3·10 ⁻⁷
2,3,6-trichlorophenol (236-CP)	933-75-5	197.45	3.45	808	2.3·10 ⁻⁷
2,4,5-trichlorophenol (245-CP)	95-95-4	197.45	3.45	808	2.3·10 ⁻⁷
2,4,6-trichlorophenol (246-CP)	88-06-2	197.45	3.45	808	2.3·10 ⁻⁷
3,4,5-trichlorophenol (345-CP)	609-19-8	197.45	3.45	808	2.3·10 ⁻⁷
2,3,4,5-tetrachlorophenol (2345-CP)	4901-51-3	231.89	4.09	193	1.7·10 ⁻⁷
2,3,4,6-tetrachlorophenol (2346-CP)	58-90-2	231.89	4.09	193	1.7·10 ⁻⁷
2,3,5,6-tetrachlorophenol (2356-CP)	935-95-5	231.89	4.09	193	1.7·10 ⁻⁷
Pentachlorophenol* (PCP)	87-86-5	266.34	4.74	45	1.3·10 ⁻⁷
4-Nonylphenol* (4NP)	84852-15-3	220.36	5.92	2.7	6.0·10 ⁻⁶
Butylhydroxytoluene (BHT)	128-37-0	220.36	5.03	10	4.1·10 ⁻⁶
Triclosan (TCS)	3380-34-5	289.55	4.66	9.3	5.0·10 ⁻⁹
Chlorobenzenes					
Polychlorobenzenes (PBCz)					
1,2-dichlorobenzene (12CBz)	95-50-1	147.00	3.28	104	3.0·10 ⁻³
1,3-dichlorobenzene (13CBz)	541-73-1	147.00	3.28	104	3.0·10 ⁻³
1,4-dichlorobenzene (14CBz)	106-46-7	147.00	3.28	104	3.0·10 ⁻³
1,2,3-trichlorobenzene* (123CBz)	87-61-6	181.45	3.93	26	2.2·10 ⁻³
1,2,4-trichlorobenzene* (124CBz)	120-82-1	181.45	3.93	26	2.2·10 ⁻³
1,3,5-trichlorobenzene* (135CBz)	108-70-3	181.45	3.93	26	2.2·10 ⁻³
1,2,3,4-tetrachlorobenzene (1234CBz)	634-66-2	215.89	4.57	6.3	1.6·10 ⁻³
1,2,3,5-tetrachlorobenzene (1235CBz)	634-90-2	215.89	4.57	6.3	1.6·10 ⁻³
1,2,4,5-tetrachlorobenzene (1245CBz)	95-94-3	215.89	4.57	6.3	1.6·10 ⁻³
Pentachlorobenzene*, ** (PCBz)	608-93-5	250.34	5.22	1.5	1.2·10 ⁻³
Hexachlorobenzene*, ** (HCBz)	118-74-1	284.78	5.86	0.3	8.9·10 ⁻⁴
Esters					

Organophosphorus compounds (OPs)					
Tributyl phosphate (TBP)	126-73-8	266.32	3.82	101	$3.2 \cdot 10^{-6}$
Triphenyl phosphate (TPP)	115-86-6	326.29	4.70	4.7	$4.0 \cdot 10^{-8}$
Tris(2-chloroethyl) phosphate (TCEP)	115-96-8	285.49	1.63	5 597	$2.6 \cdot 10^{-8}$
Tris(2-chloroisopropyl) phosphate (TCPP)	13674-84-5 ^f	327.57	2.89	740	$6.0 \cdot 10^{-8}$
Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	13674-87-8	430.91	3.65	30	$2.6 \cdot 10^{-9}$
Tris(2-butoxyethyl) phosphate (TBEP)	78-51-3	398.48	3.00	604	$1.2 \cdot 10^{-11}$
Phthalates					
Dimethyl phthalate (DMP)	131-11-3	194.19	1.66	7 459	$2.2 \cdot 10^{-7}$
Diethyl phthalate (DEP)	84-66-2	222.24	2.65	720	$3.9 \cdot 10^{-7}$
Di- <i>n</i> -butyl phthalate (DBP)	84-74-2	278.35	4.61	6.4	$1.2 \cdot 10^{-6}$
Butylbenzyl phthalate (BBP)	85-68-7	312.37	4.84	1.1	$4.2 \cdot 10^{-8}$
Di-(2-ethylhexyl) phthalate (DEHP)*	117-81-7	390.57	8.39	$1.3 \cdot 10^{-3}$	$1.2 \cdot 10^{-5}$
Di- <i>n</i> -octyl phthalate (DNOP)	117-84-0	390.57	8.54	$4.5 \cdot 10^{-4}$	$1.2 \cdot 10^{-5}$
Di- <i>iso</i> -decyl phthalate (DIDP)	26761-40-0	446.68	10.36	$1.0 \cdot 10^{-5}$	$3.7 \cdot 10^{-5}$
	68515-49-1				
Di- <i>iso</i> -nonyl phthalate (DINP)	28553-12-0	418.62	9.37	$1.2 \cdot 10^{-4}$	$2.1 \cdot 10^{-5}$
	68515-48-0				
Adipates (not included in the PCA model)					
Diethyl adipate	141-28-6	202.25	2.37	695	$1.7 \cdot 10^{-6}$
Di- <i>iso</i> -butyl adipate	141-04-8	258.36	4.19	18	$5.4 \cdot 10^{-6}$
Dibutyl adipate	105-99-7	258.36	4.33	6.31	$5.4 \cdot 10^{-6}$
Di-(2-ethylhexyl) adipate	103-23-1	370.58	8.12	$1.3 \cdot 10^{-3}$	$5.2 \cdot 10^{-5}$
Dioctyl adipate	123-79-5	370.58	8.26	$4.6 \cdot 10^{-4}$	$5.2 \cdot 10^{-5}$
Didecyl adipate	105-97-5	426.69	10.23	$3.8 \cdot 10^{-6}$	$1.6 \cdot 10^{-4}$
Di- <i>iso</i> -octyl adipate	1330-86-5	370.58	8.12	$1.3 \cdot 10^{-3}$	$5.2 \cdot 10^{-5}$
Di- <i>iso</i> -decyl adipate	27178-16-1	426.69	10.08	$1.1 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$
Antibiotics					
Fluoroquinolones (FQs)					
Norfloxacin (Nor)	70458-96-7	319.34	-0.31	40 231	$8.7 \cdot 10^{-19}$
Ofloxacin (Ofi)	82419-36-1	361.38	-0.20	6 873	$5.0 \cdot 10^{-20}$
Ciprofloxacin (Cip)	85721-33-1	331.35	0.28 ^g	19 440	$5.1 \cdot 10^{-19}$
Tetracyclines (not included in the PCA model)					
Oxytetracycline	2058-46-0	450.88	-3.60	156	$1.7 \cdot 10^{-30}$
Tetracycline	64-75-5	482.92	-3.70	$3.4 \cdot 10^5$	$1.3 \cdot 10^{-31}$
Demeclocycline	127-33-3	464.86	-1.14	$8.6 \cdot 10^4$	$2.6 \cdot 10^{-24}$
Chlorotetracycline	57-62-5	478.89	-0.68	$3.8 \cdot 10^4$	$3.5 \cdot 10^{-24}$
Doxycycline	564-25-0	444.44	-1.36	$1.2 \cdot 10^5$	$4.7 \cdot 10^{-24}$
Pharmaceuticals (not included in the PCA model)					
Non-steroid anti-inflammatory drugs (NSAIDs)					
Ibuprofen	15687-27-1	206.29	3.79	58	$1.5 \cdot 10^{-7}$
Naproxen	22204-53-1	230.27	3.10	44	$3.4 \cdot 10^{-10}$
Ketoprofen	22071-15-4	254.29	3.00	256	$2.1 \cdot 10^{-11}$
Diclofenac	15307-86-5	296.15	4.02	11	$4.7 \cdot 10^{-12}$

Hormones					
Estriol	50-27-1	288.39	2.81	558	$1.3 \cdot 10^{-12}$
Estradiol	50-28-2	272.39	3.94	50	$3.6 \cdot 10^{-11}$
Ethinylestradiol	57-63-6	296.41	4.12	13	$7.9 \cdot 10^{-12}$
Norethindrone	68-22-4	298.43	2.99	30	$5.8 \cdot 10^{-10}$

Dioxin-like compounds

Polychlorinated biphenyls (WHO-PCBs)**					
PCB 77	32598-13-3	291.99	6.34	$3.2 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$
PCB 81	70362-50-4	291.99	6.34	$3.2 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$
PCB 126	57465-28-8	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 169	32774-16-6	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 105	32598-14-4	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 114	74472-37-0	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 118 ^h	31508-00-6	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 123	65510-44-3	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 156	38380-08-4	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 157	69782-90-7	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 167	52663-72-6	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 189	39635-31-9	395.33	8.27	$3.7 \cdot 10^{-4}$	$5.1 \cdot 10^{-5}$
Polychlorinated dibenzo-<i>p</i>-dioxins and -furans (PCDD/Fs)**					
2,3,7,8-TCDD (2378-CDD)	1746-01-6	321.98	6.92	$3.8 \cdot 10^{-3}$	$3.5 \cdot 10^{-6}$
1,2,3,7,8-PeCDD (12378-CDD)	40321-76-4	356.42	7.56	$8.5 \cdot 10^{-4}$	$2.6 \cdot 10^{-6}$
1,2,3,4,7,8-HxCDD (123478-CDD)	39227-28-6	390.87	8.21	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-6}$
1,2,3,6,7,8-HxCDD (123678-CDD)	57653-85-7	390.87	8.21	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-6}$
1,2,3,7,8,9-HxCDD (123789-CDD)	19408-74-3	390.87	8.21	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-6}$
1,2,3,4,6,7,8-HpCDD (1234678-CDD)	35822-46-9	425.31	8.85	$4.2 \cdot 10^{-5}$	$1.4 \cdot 10^{-6}$
OCDD	3268-87-9	459.76	9.50	$9.3 \cdot 10^{-6}$	$1.1 \cdot 10^{-6}$
2,3,7,8-TCDF (2378-CDF)	51207-31-9	305.98	6.29	$3.1 \cdot 10^{-2}$	$1.5 \cdot 10^{-5}$
1,2,3,7,8-PeCDF (12378-CDF)	57117-41-6	340.42	6.94	$6.9 \cdot 10^{-3}$	$1.1 \cdot 10^{-5}$
2,3,4,7,8-PeCDF (23478-CDF)	57117-31-4	340.42	6.94	$6.9 \cdot 10^{-3}$	$1.1 \cdot 10^{-5}$
1,2,3,4,7,8-HxCDF (123478-CDF)	70648-26-9	374.87	7.92	$3.5 \cdot 10^{-4}$	$6.8 \cdot 10^{-6}$
1,2,3,6,7,8-HxCDF (123678-CDF)	57117-44-9	374.87	7.92	$3.5 \cdot 10^{-4}$	$6.8 \cdot 10^{-6}$
2,3,4,6,7,8-HxCDF (234678-CDF)	60851-34-5	374.87	7.92	$3.5 \cdot 10^{-4}$	$6.8 \cdot 10^{-6}$
1,2,3,7,8,9-HxCDF (123789-CDF)	72918-21-9	374.87	7.58	$1.6 \cdot 10^{-3}$	$8.5 \cdot 10^{-6}$
1,2,3,4,6,7,8-HpCDF (1234678-CDF)	67562-39-4	409.31	8.23	$3.5 \cdot 10^{-4}$	$6.3 \cdot 10^{-6}$
1,2,3,4,7,8,9-HpCDF (1234789-CDF)	55673-89-7	409.31	8.23	$3.5 \cdot 10^{-4}$	$6.3 \cdot 10^{-6}$
OCDF	39001-02-0	443.76	8.87	$7.6 \cdot 10^{-5}$	$4.7 \cdot 10^{-6}$

Other organic compounds

Polycyclic aromatic hydrocarbons (PAHs)* (PAHsum)

Fluoranthene	206-44-0	202.26	4.93	$9.1 \cdot 10^{-2}$	$8.3 \cdot 10^{-6}$
Benzo(b)fluoranthene	205-99-2	252.32	6.11	$2.0 \cdot 10^{-3}$	$8.1 \cdot 10^{-7}$
Benzo(k)fluoranthene	207-08-9	252.32	6.11	$2.0 \cdot 10^{-3}$	$8.1 \cdot 10^{-7}$
Benzo(a)pyrene	50-32-8	252.32	6.11	$2.0 \cdot 10^{-3}$	$8.1 \cdot 10^{-7}$
Benzo(g,h,i)perylene	191-24-2	276.34	6.70	$1.8 \cdot 10^{-4}$	$1.3 \cdot 10^{-7}$
Indeno(1,2,3-cd)pyrene	193-39-5	276.34	6.70	$1.8 \cdot 10^{-4}$	$1.3 \cdot 10^{-7}$

Polychlorinated biphenyls (Indicator-PCBs)** (PCB7)

PCB 28	7012-37-5	257.55	5.69	0.14	$1.7 \cdot 10^{-4}$
PCB 52	35693-99-3	291.99	6.34	$3.2 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$
PCB 101	37680-73-2	236.44	6.98	$7.3 \cdot 10^{-2}$	$9.2 \cdot 10^{-5}$
PCB 118 ^h	31508-00-6	326.44	6.98	$7.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-5}$
PCB 138	35065-28-2	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 153	35065-27-1	360.88	7.62	$1.6 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$
PCB 180	35065-29-3	395.33	8.27	$3.7 \cdot 10^{-4}$	$5.1 \cdot 10^{-5}$

Polybrominated diphenylethers (PBDEs)

PBDE 28*	41318-75-6	406.90	5.88	0.27	$7.5 \cdot 10^{-6}$
PBDE 47*, **	5436-43-1	485.79	6.77	$5.4 \cdot 10^{-2}$	$3.0 \cdot 10^{-6}$
PBDE 99*, **	60348-60-9	564.69	7.66	$1.1 \cdot 10^{-2}$	$1.2 \cdot 10^{-6}$
PBDE 100*, **	189084-64-8	564.69	7.66	$1.1 \cdot 10^{-2}$	$3.0 \cdot 10^{-6}$
PBDE 153*, **	68631-49-2	643.59	8.55	$2.1 \cdot 10^{-3}$	$1.2 \cdot 10^{-6}$
PBDE 154*, **	207122-15-4	643.59	8.55	$2.1 \cdot 10^{-3}$	$1.5 \cdot 10^{-6}$
PBDE 183**	207122-16-5	722.48	9.44	$3.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-7}$
PBDE 209	1163-19-5	959.17	12.11	$2.6 \cdot 10^{-6}$	$1.2 \cdot 10^{-8}$

Polychlorinated alkanes (PCAs)

SCCP*	85535-84-8	Physicochemical properties depend on the degree of chlorination			
MCCP	85535-85-9				
LCCP	85422-92-0				

Siloxanes (not included in the PCA model)

Octamethylcyclotetrasiloxane	556-67-2	296.62	5.09	0.17	$8.7 \cdot 10^{-2}$
Decamethylcyclopentasiloxane	541-02-6	370.78	5.71	$1.9 \cdot 10^{-2}$	0.12
Dodecamethylcyclohexasiloxane	540-97-6	444.93	6.33	$2.1 \cdot 10^{-3}$	0.17
Hexamethyldisiloxane	107-46-0	162.39	4.76	1.36	0.30
Octamethyltrisiloxane	107-51-7	236.54	5.35	$6.4 \cdot 10^{-2}$	0.42
Decamethyltetrasiloxane	141-62-8	310.69	5.93	$2.7 \cdot 10^{-3}$	0.57
Dodecamethyltetrasiloxane	141-63-9	384.85	6.52	$1.1 \cdot 10^{-4}$	0.79

Terpenes (not included in the PCA model)

D-limonene	5989-27-5	136.24	4.83	44	0.38
L-limonene	5989-54-8	136.24	4.83	44	0.38

Fluorinated compounds

Perfluorochemicals (PFCs)

Perfluorohexane acid (PFHxA)	307-24-4	314.06	4.37	0.85	$3.3 \cdot 10^{-3}$
Perfluoroheptane acid (PFHpA)	375-85-9	364.06	5.33	$4.2 \cdot 10^{-2}$	$1.7 \cdot 10^{-2}$
Perfluorooctane acid (PFOA)	335-67-1	414.07	6.30	$2.1 \cdot 10^{-3}$	$9.1 \cdot 10^{-2}$
Perfluorononane acid (PFNA)	375-95-1	464.08	7.27	$9.9 \cdot 10^{-5}$	0.48
Perfluorodecane acid (PFDA)	335-76-2	514.09	8.23	$4.7 \cdot 10^{-6}$	2.5
Perfluoroundecane acid (PFUnA)	2058-94-8	564.10	9.20	$5.6 \cdot 10^{-7}$	13
Perfluorododecane acid (PFDoDA)	307-55-1	614.10	10.16	$6.1 \cdot 10^{-7}$	69
Perfluorotridecane acid (PFTrDA)	376-03-4	664.11	n.e.	n.e.	n.e.
Perfluorotetradecane acid (PFTeDA)	376-06-7	714.12	12.10	$7.1 \cdot 10^{-7}$	$1.9 \cdot 10^3$
Perfluorohexane sulfonate (PFHxS)	3871-99-6	438.20	2.20	$3.4 \cdot 10^{-3}$	n.e.
Perfluorooctane sulfonate (PFOS)**	2795-39-3	538.22	4.13	$7.6 \cdot 10^{-6}$	n.e.
Perfluorodecane sulfonate (PFDS)	335-77-3	600.14	8.21	$1.1 \cdot 10^{-4}$	$3.0 \cdot 10^{-1}$
Perfluorooctane sulfonamide (PFOSA)	4151-50-2	527.20	8.54	$1.5 \cdot 10^{-4}$	5.4

Organometals

Organotin compounds (OTCs)

Monobutyltin (MBT)	78763-54-9 ⁱ	176.83	3.31	3 668	$9.7 \cdot 10^{-2}$
Dibutyltin (DBT)	1002-53-5	232.94	0.57	56	0.38
Tributyltin* (TBT)	688-73-3 ^j	291.07	7.35	0.8	1.5
Monophenyltin (MPhT)	n.e.	196.82	3.05	2 109	$3.6 \cdot 10^{-3}$
Diphenyltin (DPHT)	1135-99-5 ^k	272.92	1.76	18	$5.3 \cdot 10^{-4}$
Triphenyltin (TPHT)	668-34-8 ^l	351.04	6.58	0.14	$7.8 \cdot 10^{-5}$

Metals

As	7440-38-2	77.95	0.68	$1.4 \cdot 10^5$	0.77
Cd*	7440-43-9	112.41	-0.07	$2.0 \cdot 10^5$	$2.5 \cdot 10^{-2}$
Co	7440-48-4	58.93	0.23	$1.1 \cdot 10^5$	$2.5 \cdot 10^{-2}$
Cr	7440-47-3	52.00	0.23	$9.2 \cdot 10^4$	$2.5 \cdot 10^{-2}$
Cu	7440-50-8	63.55	-0.57	$1.1 \cdot 10^5$	$2.5 \cdot 10^{-2}$
Hg*	7439-97-6	200.59	0.62	$6.4 \cdot 10^4$	$2.5 \cdot 10^{-2}$
Ni*	7440-02-0	58.69	-0.57	$1.0 \cdot 10^5$	$2.5 \cdot 10^{-2}$
Pb*	7439-92-1	207.2	0.73	$3.7 \cdot 10^5$	$2.5 \cdot 10^{-2}$
V	7440-62-2	50.94	0.23	$9.0 \cdot 10^4$	$2.5 \cdot 10^{-2}$
Zn	7440-66-6	67.41	-0.47	$1.2 \cdot 10^5$	$2.5 \cdot 10^{-2}$

Pesticides (not included in the PCA model)

Insecticides

Acephate	30560-19-1	183.16	-0.90	$1.0 \cdot 10^6$	$2.8 \cdot 10^{-12}$
α -cypermethrine	67375-30-8	416.31	6.38	$1.7 \cdot 10^{-2}$	$7.9 \cdot 10^{-7}$
Aldrin**	309-00-2	364.92	6.75	$2.4 \cdot 10^{-3}$	$3.9 \cdot 10^{-4}$
Azinophosmethyl	86-50-0	317.32	2.53	150	$2.9 \cdot 10^{-10}$
Bromopropylate	18181-80-1	428.12	4.90	5.1	$5.0 \cdot 10^{-8}$
Cyfluthrin	68359-37-5	434.30	5.74	$1.5 \cdot 10^{-2}$	$9.2 \cdot 10^{-7}$
β -cyfluthrin	68359-37-5	434.30	5.74	$1.5 \cdot 10^{-2}$	$9.2 \cdot 10^{-7}$
Cypermethrine	52315-07-8	416.31	6.38	$1.7 \cdot 10^{-2}$	$7.9 \cdot 10^{-7}$
DDD-p,p	72-54-8	320.05	5.87	$2.0 \cdot 10^{-2}$	$4.3 \cdot 10^{-5}$
DDE-p,p	72-55-9	318.03	6.00	$4.0 \cdot 10^{-2}$	$3.5 \cdot 10^{-5}$
DDT-o,p**	789-02-6	354.49	6.79	$3.4 \cdot 10^{-3}$	$1.5 \cdot 10^{-5}$
DDT-p,p**	50-29-3	354.49	6.79	$3.4 \cdot 10^{-3}$	$1.5 \cdot 10^{-5}$
Deltamethrine	52918-63-5	505.21	6.18	$4.3 \cdot 10^{-2}$	$6.1 \cdot 10^{-8}$
Diazinon	333-41-5	304.35	3.86	110	$8.7 \cdot 10^{-8}$

Dieldrin**	60-57-1	380.91	5.45	$2.2 \cdot 10^{-2}$	$5.4 \cdot 10^{-7}$
Dichlorvos	62-73-7	220.98	0.60	$1.5 \cdot 10^5$	$8.6 \cdot 10^{-7}$
Dimethoate	60-51-5	229.25	0.28	$1.4 \cdot 10^5$	$2.1 \cdot 10^{-11}$
α -endosulfan*, **	959-98-8	406.92	3.50	0.38	$9.0 \cdot 10^{-8}$
β -endosulfan**	33213-65-9	406.92	3.50	0.38	$9.0 \cdot 10^{-8}$
Endosulfan sulfate	1031-07-8	422.92	3.64	0.48	$1.1 \cdot 10^{-8}$
Carbaryl	63-25-2	201.23	2.35	210	$3.1 \cdot 10^{-9}$
Carbophenothion	786-19-6	342.86	5.19	0.21	$1.8 \cdot 10^{-7}$
Carbofuran	1563-66-2	221.26	2.30	220	$1.6 \cdot 10^{-9}$
Carbosulfan	55285-14-8	380.55	5.57	0.69	$2.2 \cdot 10^{-9}$
Keto-endrin	53494-70-5	380.91	4.99	$7.5 \cdot 10^{-2}$	$2.0 \cdot 10^{-8}$
α -chlordane**	5103-71-9	409.78	6.26	$3.8 \cdot 10^{-3}$	$7.0 \cdot 10^{-5}$
γ -chlordane**	5566-34-7	409.78	7.00	$1.8 \cdot 10^{-3}$	$7.0 \cdot 10^{-5}$
Chlorfenvinphos*	470-90-6	359.58	4.15	20	$5.2 \cdot 10^{-8}$
Chlorobenzilate	510-15-6	325.19	3.99	12	$1.3 \cdot 10^{-7}$
Chlorpyrifos*	2921-88-2	350.59	4.66	11	$2.5 \cdot 10^{-6}$
λ -cyhalotrin	91465-08-6	449.86	6.85	$2.1 \cdot 10^{-3}$	$1.4 \cdot 10^{-5}$
Methidathion	950-37-8	302.32	1.58	$1.7 \cdot 10^4$	$7.1 \cdot 10^{-9}$
Methoxychlor	72-43-5	345.66	5.67	$1.8 \cdot 10^{-2}$	$9.8 \cdot 10^{-8}$
Parathion ethyl	56-38-2	291.26	3.73	8.4	$3.0 \cdot 10^{-7}$
Parathion methyl	298-00-0	263.21	2.75	90	$1.7 \cdot 10^{-7}$
Permethrine	52645-53-1	391.30	7.43	$2.4 \cdot 10^{-3}$	$2.9 \cdot 10^{-7}$
Pirimicarb	23103-98-2	238.29	1.40	$1.4 \cdot 10^4$	$2.6 \cdot 10^{-9}$
Pirimiphos methyl	29232-93-7	305.33	3.44	240	$2.5 \cdot 10^{-6}$
Endrin**	72-20-8	380.91	5.45	$2.2 \cdot 10^{-2}$	$5.4 \cdot 10^{-7}$
Esfenvalerate	66230-04-4	419.91	6.76	$6.2 \cdot 10^{-3}$	$1.2 \cdot 10^{-7}$
Fensulfothion	115-90-2	308.35	2.35	$2.0 \cdot 10^3$	$1.4 \cdot 10^{-10}$
Fenvalerate	51630-58-1	419.91	6.76	$6.2 \cdot 10^{-3}$	$1.2 \cdot 10^{-7}$
Flucythrinate	70124-77-5	451.47	6.56	$4.6 \cdot 10^{-3}$	$3.8 \cdot 10^{-8}$
α -HCH*, **	319-84-6	290.83	4.26	6.6	$2.6 \cdot 10^{-4}$
β -HCH*, **	319-85-7	290.83	4.26	6.6	$2.6 \cdot 10^{-4}$
δ -HCH*, **	319-86-8	290.83	4.26	6.6	$2.6 \cdot 10^{-4}$
γ -HCH (Lindane)*	58-89-9	290.83	4.26	6.6	$2.6 \cdot 10^{-4}$
Heptachlor**	76-44-8	373.32	5.86	$9.2 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$
Heptachlorepoxyde	1024-57-3	389.32	4.56	$8.4 \cdot 10^{-2}$	$2.5 \cdot 10^{-7}$
Propargite	2312-35-8	350.48	5.57	0.50	$9.2 \cdot 10^{-8}$
Propoxur	114-26-1	209.25	1.90	810	$3.4 \cdot 10^{-9}$
Pyridaben	96489-71-3	364.94	5.47	0.46	$2.3 \cdot 10^{-10}$
Quinalphos	13593-03-8	298.30	3.04	150	$4.0 \cdot 10^{-9}$
Tetradiphone	116-29-0	356.05	5.18	$2.6 \cdot 10^{-2}$	$7.5 \cdot 10^{-8}$
Herbicides					
Glyphosate	1071-83-6	169.07	-4.47	$1.0 \cdot 10^6$	$4.1 \cdot 10^{-19}$
Aminomethylphosphonic acid	1066-51-9	111.04	-2.17	$1.0 \cdot 10^6$	$1.3 \cdot 10^{-15}$
Aclonifen	74070-46-5	264.67	3.88	5.7	$2.7 \cdot 10^{-9}$
Alachlor*	15972-60-8	269.77	3.37	440	$2.2 \cdot 10^{-8}$
Atrazine*	1912-24-9	215.69	2.82	45	$4.5 \cdot 10^{-9}$
Desethylatrazine	6190-65-4	187.63	1.78	280	$1.5 \cdot 10^{-9}$
Desisopropylatrazine	1007-28-9	173.61	1.36	540	$1.2 \cdot 10^{-9}$
Cinidon ethyl	142891-20-1	n.e.	n.e.	n.e.	n.e.
Cyanazine	21725-46-2	240.70	2.51	96	$1.9 \cdot 10^{-12}$
Diflufenican	83164-33-4	394.30	3.53	1.6	$3.8 \cdot 10^{-12}$
Dichlorobenil	1194-65-6	172.01	2.83	36	$2.9 \cdot 10^{-5}$
Diuron*	330-54-1	233.10	2.67	100	$5.3 \cdot 10^{-10}$
Isoproturon*	34123-59-6	206.29	2.84	92	$1.9 \cdot 10^{-9}$
Carfentrazone ethyl	128639-02-1	412.20	4.26	0.30	$6.0 \cdot 10^{-11}$
Chloridazon	1698-60-8	221.65	0.76	$3.4 \cdot 10^4$	$6.5 \cdot 10^{-12}$

Chlorpropham	101-21-3	213.67	3.30	49	$2.9 \cdot 10^{-8}$
Metabenzthiazuron	18691-97-9	221.28	2.65	$1.1 \cdot 10^3$	$6.3 \cdot 10^{-13}$
Metamitron	41394-05-2	202.22	1.44	$4.0 \cdot 10^4$	$5.9 \cdot 10^{-12}$
Methazachlor	67129-08-2	277.79	2.38	670	$5.8 \cdot 10^{-11}$
Metribuzin	21087-64-9	214.29	1.49	$2.1 \cdot 10^5$	$1.8 \cdot 10^{-12}$
Pendimethaline	40487-42-1	281.31	4.82	0.77	$1.5 \cdot 10^{-6}$
Ethofumesate	26225-79-6	286.35	2.89	12	$1.2 \cdot 10^{-9}$
Phenmedipham	13684-63-4	300.32	3.27	0.68	$5.7 \cdot 10^{-11}$
Flurtamone	96525-23-4	333.31	2.87	35	$1.7 \cdot 10^{-9}$
Hexazinone	51235-04-2	252.32	2.15	590	$4.1 \cdot 10^{-13}$
Propyzamide	23950-58-5	256.13	3.57	41	$1.0 \cdot 10^{-9}$
Prosulfocarb	52888-80-9	251.39	4.23	5.7	$9.4 \cdot 10^{-7}$
Simazine*	122-34-9	201.66	2.40	86	$3.4 \cdot 10^{-9}$
Terbutylazine desethyl*	134-62-3	191.28	2.26	170	$2.1 \cdot 10^{-8}$
Terbutryn	886-50-0	241.36	3.77	42	$9.1 \cdot 10^{-9}$
Terbutylazine	5915-41-3	229.71	3.27	20	$5.9 \cdot 10^{-9}$
Trifluralin*	1582-09-8	335.29	5.31	$5.5 \cdot 10^{-2}$	$2.1 \cdot 10^{-4}$
Fungicides					
Azoxystrobin	131860-33-8	403.40	1.58	94	$8.0 \cdot 10^{-14}$
BAM (2,6-dichlorobenzamide)	2008-58-4	190.03	0.90	$1.2 \cdot 10^3$	$1.2 \cdot 10^{-9}$
Bitertanol	55179-31-2	337.42	4.07	42	$1.6 \cdot 10^{-12}$
Cyprodinil	121552-61-2	225.30	3.99	12	$1.9 \cdot 10^{-6}$
Diphenylamine	122-39-4	169.23	3.29	55	$1.1 \cdot 10^{-6}$
Captan	133-06-2	300.59	2.74	700	$4.6 \cdot 10^{-9}$
Chlorothalonil	1897-45-6	265.91	3.66	0.68	$1.5 \cdot 10^{-7}$
Quintozene	82-68-8	295.34	5.03	0.71	$4.8 \cdot 10^{-6}$
Pentachloroaniline	527-20-8	265.35	1.70	$9.2 \cdot 10^3$	$8.1 \cdot 10^{-10}$
Metalaxyl	57837-19-1	279.34	4.30	19	$4.3 \cdot 10^{-7}$
Prochloraz	67747-09-5	376.67	4.13	3.0	$7.6 \cdot 10^{-12}$
Fenpropimorph	67306-03-0	303.49	5.50	5.3	$2.2 \cdot 10^{-7}$
Heptachlorobenzene* **	116-74-1	n.e.	n.e.	n.e.	n.e.
Imazalil	35554-44-0	297.19	4.10	9.8	$7.3 \cdot 10^{-8}$
Iprodione	36734-19-7	330.17	2.85	$3.8 \cdot 10^{-2}$	$1.0 \cdot 10^{-13}$
Propiconazole	60207-90-1	342.23	4.13	11	$1.4 \cdot 10^{-9}$
Pyraclostrobin	175013-18-0	n.e.	n.e.	n.e.	n.e.
Pyrimethanil	53112-28-0	199.26	3.19	78	$2.5 \cdot 10^{-6}$
Spiroxamine	118134-30-8	297.49	5.51	25	$1.9 \cdot 10^{-7}$
Thiabendazole	148-79-8	201.25	2.00	480	$2.0 \cdot 10^{-11}$
Tolchlofosmethyl	57018-04-9	301.13	4.77	3.2	$2.6 \cdot 10^{-5}$
Tolyfluanid	731-27-1	347.25	3.27	64	$7.4 \cdot 10^{-7}$
Vinclozolin	50471-44-8	286.12	3.03	2.1	$2.4 \cdot 10^{-6}$

	Biocides				
2-Mercaptobenzothiazole (2MERCAPTOB)	149-30-4	167.24	2.86	110	$3.6 \cdot 10^{-8}$
2-(Tiocyanomethylthio)benzothiazole (2TIOCYANOM)	21564-17-0	238.34	3.12	59	$6.5 \cdot 10^{-12}$
4-Chloro-3-cresol (KLORKRESOL)	59-50-7	142.59	2.70	$4.2 \cdot 10^3$	$4.6 \cdot 10^{-7}$
N-didecyldimethylammonium chloride (DDMAC)	7173-51-5	362.09	4.66	$7.2 \cdot 10^{-6}$	$6.9 \cdot 10^{-10}$
Propiconazole (PROPICONA)	60207-90-1	342.23	4.13	11	$1.4 \cdot 10^{-9}$
Resorcinol (RESORCINOL)	108-46-3	110.11	1.03	$3.1 \cdot 10^5$	$5.8 \cdot 10^{-11}$
Methylparabene (MEPARAB)	99-76-3	152.15	2.00	$4.3 \cdot 10^3$	$3.6 \cdot 10^{-9}$
Ethylparabene (ETPARAB)	120-47-8	166.18	2.49	$1.4 \cdot 10^3$	$4.8 \cdot 10^{-9}$
Propylparabene (PROPARAB)	94-13-3	180.21	2.98	425	$6.4 \cdot 10^{-9}$
Butylparabene (BUPARAB)	94-26-8	194.23	3.47	133	$8.5 \cdot 10^{-9}$
Benzylparabene (BEPARAB)	94-18-8	228.25	3.70	23	$2.9 \cdot 10^{-10}$

^aCAS RN, Chemical Abstracts Service Registry Number. ^bM_w, Molecular weight. ^clog K_{ow}, octanol-water partition coefficient, estimated values. ^dS_w, Water Solubility. ^eatm·m³ mol⁻¹. ^fThe commercial mixture contains four isomers, of which tris(2-chloroisopropyl) phosphate is the most abundant. ^gexperimental value (Takacs-Novak et al., 1992). ^hPCB 118 is classified both as WHO- and Indicator-PCB. ⁱMonobutyltin ion.

^jTributyltin hydride. ^kDiphenyltin ion. ^lTriphenyltin ion.

Table S2 Comparative data of the analytical techniques and quantifying uncertainties in the analyses of the compounds

Class of compound	Sub group	Analytical technique ^a	Quantifying uncertainty (%)	Reference
Phenols	Chlorophenols	GC-MS	± 20	CL ^{b,c}
	Butylhydroxytoluene	GC-MS	± 20	CL ^{d,e}
	Triclosan	GC-MS	± 20	CL ^d
	4-Nonylphenol	GC-MS	± 40	CL ^c
Chlorobenzenes	Polychlorobenzenes	GC-MS	± 30	(Liljelind et al., 2003) ^d
Esters	Organophosphorus compounds	GC-MS	± 30	(Marklund et al., 2005) ^d
	Phthalates	GC-MS	± 20	CL ^d
	Adipates	GC-MS	± 40	(IVL, 2005a)
Antibiotics	Fluoroquinolones	LC-MS/MS	± 20	(Lindberg et al., 2005) ^d
	Tetracyclines	LC-TOF-MS	± 40	(IVL, 2006a)
Pharmaceuticals	NSAIDs	GC-MS	± 40	(IVL, 2006a)
	Hormones	LC-TOF-MS	± 40	(IVL, 2006a)
Dioxin-like compounds	WHO-PCBs	GC-HRMS	± 29	(Liljelind et al., 2003) ^c
	PCDD/Fs	GC-HRMS	± 29	(Liljelind et al., 2003) ^c
Other POPs	Polycyclic aromatic hydrocarbons	GC-MS	± 30	(Swedish EPA, 1990) ^c
	Indicator-PCBs	GC-MS	± 40	(Swedish EPA, 1990) ^c
	Polybrominated diphenylethers	GC-MS	± 30	(Liljelind et al., 2003) ^d
	Chloroparaffins	GC-MS	± 30	(Reth et al., 2005) ^{d,f}
	Siloxanes	ATD-GC-MS	± 40	(IVL, 2005b)
	Terpene (Limonene)	ATD-GC-FID	± 40	(IVL, 2005c)
Fluorinated compounds	Perfluorochemicals	LC-MS/MS	± 5-20	(Karrman et al., 2005) ^g
Organometals	Organotin compounds	ICP-MS	± 6-40	(Kumar et al., 2003) ^d
Metals	As, Cd, Co, Cr, Hg, Ni, Pb	ICP- SFMS	± 20	(U.S.EPA, 1994a) ^c
	Cu, V, Zn	ICP- AES	± 20-30	(U.S.EPA, 1994b) ^c
Pesticides	Insecticides, herbicides, and fungicides	GC-MS	± 40	CL ^d
Biocides		GC-MS	± 40	(IVL, 2006b)

^aGC, 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. ^bCL, Commercial Laboratory. ^cAccredited analysis.

^dIn-house validated analytical method. ^eBHT semi-quantitatively analyzed, the results are presented in benzylbenzoate-equivalents. ^fModification: ¹³C labelled PCB 188 was used as recovery standard instead of ε-HCH. ^gWith some modifications.

Table S3 Concentrations of the metals, persistent organic pollutants (POPs), pharmaceuticals and personal care products (PPCPs), and other organic contaminants in sewage sludge

*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

Chemical	STP A	STP B	STP C	STP D	STP E	STP F	STP G
Phenols							
Chlorophenols (CPs)	<i>mg kg⁻¹ d.w.</i>						
2-monochlorophenol (2-CP)	0.022	<0.02	<0.02	<0.02	<0.02	0.028	0.036
3-monochlorophenol (3-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
4-monochlorophenol (4-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3-dichlorophenol (23-CP)	0.022	<0.02	<0.02	<0.02	<0.02	0.028	0.036
2,4-dichlorophenol (24-CP)+							
2,5-dichlorophenol (25-CP)	0.042	0.07	0.034	<0.02	0.062	0.021	0.064
2,6-dichlorophenol (26-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
3,4-dichlorophenol (34-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
3,5-dichlorophenol (35-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,4-trichlorophenol (234-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,5-trichlorophenol (235-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,6-trichlorophenol (236-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,4,5-trichlorophenol (245-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,4,6-trichlorophenol (246-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
3,4,5-trichlorophenol (345-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,4,5-tetrachlorophenol (2345-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,4,6-tetrachlorophenol (2346-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
2,3,5,6-tetrachlorophenol (2356-CP)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Pentachlorophenol* (PCP))	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.04
4-Nonylphenol* (4NP)	20	21	8	12	40	13.1	10
Butylhydroxytoluene (BHT))	0.81	0.64	0.83	1.5	2.4	1.6	2.2
Triclosan (TCS)	4.6	8.3	1.8	5.5	3.7	2.4	3.4
Chlorobenzenes							
Polychlorobenzenes (PBCz)	<i>µg kg⁻¹ d.w.</i>						
1,2-dichlorobenzene (12CBz)	7	3	<0.003	<0.003	79	2	<0.003
1,3-dichlorobenzene (13CBz) +							
1,4-dichlorobenzene (14CBz)	26	5	<0.003	14	64	29	8
1,2,3-trichlorobenzene* (123CBz)	<0.003	<0.003	149	<0.003	<0.003	<0.003	<0.003
1,2,4-trichlorobenzene* (124CBz)	<0.003	<0.003	541	<0.003	<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) +							
1,2,4,5-tetrachlorobenzene (1245CBz)	0.9	1	5	1	4	1	1
Pentachlorobenzene*’ ** (PCBz)	0.4	0.5	1	1	3	1	1
Hexachlorobenzene*’ ** (HCBz)	4	9	6	9	20	6	4

Esters							
Organophosphorus compounds (OPs)		$\mu\text{g kg}^{-1} \text{ d.w.}$					
Tributyl phosphate (TBP)	7	11	37	24	10	37	14
Triphenyl phosphate (TPP)	13	40	33	53	14	135	29
Tris(2-chloroethyl) phosphate (TCEP)	3	5	9	8	4	20	<2
Tris(2-chloroisopropyl) phosphate (TCPP)	559	409	916	859	547	1545	209
Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	24	55	22	40	32	309	56
Tris(2-butoxyethyl) phosphate (TBEP)	94	210	<32	1865	<32	<32	<32
Phthalates		$\text{mg kg}^{-1} \text{ d.w.}$					
Dimethyl phthalate (DMP)	<0.75	<0.70	<0.11	<3.2	<0.10	<0.47	<0.68
Diethyl phthalate (DEP)	<0.075	<0.07	<0.11	<0.065	<0.10	<0.047	<0.068
Di- <i>n</i> -butyl phthalate (DBP)	<0.75	<0.70	<0.11	<3.2	<0.10	<0.47	<0.68
Butylbenzyl phthalate (BBP)	<0.075	<0.07	<0.11	<0.065	<0.10	<0.047	<0.68
Di-(2-ethylhexyl) phthalate (DEHP)*	60	95	34	220	41	60	65
Di- <i>n</i> -octyl phthalate (DNOP)	<0.075	<0.07	<0.11	<0.065	<0.10	<0.047	<0.068
Di- <i>iso</i> -decyl phthalate (DIDP)	30	35	14	23	54	21	10
Di- <i>iso</i> -nonyl phthalate (DINP)	32	60	21	78	24	31	29
Adipates (not included in the PCA model)		$\mu\text{g kg}^{-1} \text{ d.w.}$					
Diethyl adipate	<5	n.m.	n.m.	n.m.	n.m.	n.m.	<5
Di- <i>iso</i> -butyl adipate	<10	n.m.	n.m.	n.m.	n.m.	n.m.	<10
Dibutyl adipate	<10	n.m.	n.m.	n.m.	n.m.	n.m.	<10
Di-(2-ethylhexyl) adipate	100	n.m.	n.m.	n.m.	n.m.	n.m.	40
Dioctyl adipate	<5	n.m.	n.m.	n.m.	n.m.	n.m.	<5
Didecyl adipate	<10	n.m.	n.m.	n.m.	n.m.	n.m.	<10
Di- <i>iso</i> -octyl adipate	<50	n.m.	n.m.	n.m.	n.m.	n.m.	<50
Di- <i>iso</i> -decyl adipate	<50	n.m.	n.m.	n.m.	n.m.	n.m.	<50
Antibiotics							
Fluoroquinolones (FQs)		$\text{mg kg}^{-1} \text{ d.w.}$					
Norfloxacin (Nor)	5.3	4.2	3.9	4.2	5.0	5.5	3.0
Ofloxacin (OfI)	1.3	1.3	<0.1	1.2	1.7	1.7	<0.1
Ciprofloxacin (Cip)	8.2	7.6	6.0	7.9	9.3	8.8	3.9
Tetracyclines (not included in the PCA model)		$\mu\text{g kg}^{-1} \text{ d.w.}$					
Oxytetracycline	<4	n.m.	1400	n.m.	n.m.	n.m.	n.m.
Tetracycline	3000	n.m.	<3	n.m.	n.m.	n.m.	n.m.
Demeclocycline	<4	n.m.	<6	n.m.	n.m.	n.m.	n.m.
Chlorotetracycline	<8	n.m.	<12	n.m.	n.m.	n.m.	n.m.
Doxycycline	1100	n.m.	<6	n.m.	n.m.	n.m.	n.m.
Pharmaceuticals (not included in the PCA model)							
Non-steroid anti-inflammatory drugs (NSAIDs)		$\mu\text{g kg}^{-1} \text{ d.w.}$					
Ibuprofen	130	n.m.	33	n.m.	n.m.	n.m.	n.m.
Naproxen	7.6	n.m.	<4	n.m.	n.m.	n.m.	n.m.
Ketoprofen	12	n.m.	<9	n.m.	n.m.	n.m.	n.m.
Diclofenac	77	n.m.	16	n.m.	n.m.	n.m.	n.m.

Hormones				<i>μg kg⁻¹ d.w.</i>			
Estriol	<1	n.m.	<2	n.m.	n.m.	n.m.	n.m.
Estradiol	<2	n.m.	<2	n.m.	n.m.	n.m.	n.m.
Ethinylestradiol	<3	n.m.	<4	n.m.	n.m.	n.m.	n.m.
Norethindrone	<6	n.m.	<9	n.m.	n.m.	n.m.	n.m.
Dioxin-like compounds							
Polychlorinated biphenyls (WHO-PCBs)**				<i>ng kg⁻¹ d.w.</i>			
PCB 77	167	97	99	99	140	89	61
PCB 81	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3
PCB 126	15	11	29	8	20	21	12
PCB 169	3	3	9	<0.6	7	4	3
PCB 105	2314	1161	841	1487	2436	2774	705
PCB 114	<2	<2	<2	<2	<2	<2	<2
PCB 118 ^h	4816	2398	2009	3227	4697	5631	1672
PCB 123	<1	<1	<1	<1	<1	<1	<1
PCB 156	1381	887	569	1152	1373	2088	605
PCB 157	504	237	285	<1	<1	<1	140
PCB 167	<1	<1	<1	<1	<1	<1	<1
PCB 189	<1	<1	<1	<1	<1	<1	<1
Polychlorinated dibenzo-<i>p</i>-dioxins and -furans (PCDD/Fs)**				<i>ng kg⁻¹ d.w.</i>			
2,3,7,8-TCDD (2378-CDD)	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
1,2,3,7,8-PeCDD (12378-CDD)	<1	<1	<1	<1	<1	<1	<1
1,2,3,4,7,8-HxCDD (123478-CDD)	<3	5	<3	<3	<3	<3	<3
1,2,3,6,7,8-HxCDD (123678-CDD)	8	6	<2	3	8	<2	<2
1,2,3,7,8,9-HxCDD (123789-CDD)	<3	<3	<3	<3	<3	<3	<3
1,2,3,4,6,7,8-HpCDD (1234678-CDD)	111	111	54	159	218	135	116
OCDD	856	844	607	1184	1224	1159	700
2,3,7,8-TCDF (2378-CDF)	6	7	4	3	8	5	4
1,2,3,7,8-PeCDF (12378-CDF)	<8	<8	<8	<8	<8	<8	<8
2,3,4,7,8-PeCDF (23478-CDF)	<3	4	<3	<3	<3	<3	<3
1,2,3,4,7,8-HxCDF (123478-CDF)	<1	<1	<1	<1	<1	<1	<1
1,2,3,6,7,8-HxCDF (123678-CDF)	<1	<1	<1	<1	<1	<1	<1
2,3,4,6,7,8-HxCDF (234678-CDF)	<1	<1	<1	<1	5	<1	<1
1,2,3,7,8,9-HxCDF (123789-CDF)	<3	<3	<3	<3	<3	<3	<3
1,2,3,4,6,7,8-HpCDF (1234678-CDF)	94	78	34	59	120	60	70
1,2,3,4,7,8,9-HpCDF (1234789-CDF)	<2	3	<2	<2	<2	<2	<2
OCDF	491	460	260	274	623	222	334

Other organic compounds

Polycyclic aromatic hydrocarbons (PAHs)* (PAHsum)		<i>mg kg⁻¹ d.w.</i>					
Fluoranthene	0.7						
Benzo(b)fluoranthene	0.3	Sum	Sum	Sum	Sum	Sum	Sum
Benzo(k)fluoranthene	0.1	PAH	PAH	PAH	PAH	PAH	PAH
Benzo(a)pyrene	0.2	<1.4	1.5	0.64	0.68	0.47	0.54
Benzo(g,h,i)perylene	0.2						
Indeno(1,2,3-cd)pyrene	0.2						
Polychlorinated biphenyls (Indicator-PCBs)** (PCB7)		<i>mg kg⁻¹ d.w.</i>					
PCB 28	0.006						
PCB 52	0.006						
PCB 101	0.009	Sum	Sum	Sum	Sum	Sum	Sum
PCB 118 ^h	0.006	PCB7	PCB7	PCB7	PCB7	PCB7	PCB7
PCB 138	0.019	<0.09	0.05	0.051	0.04	0.1	0.023
PCB 153	0.017						
PCB 180	0.009						
Polybrominated diphenylethers (PBDEs)		<i>µg kg⁻¹ d.w.</i>					
PBDE 28*	0.26	0.13	0.15	0.15	0.33	0.17	0.23
PBDE 47*, **	<0.9	20	10	72	<0.9	32	25
PBDE 99*, **	31	30	37	28	28	39	34
PBDE 100*, **	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
PBDE 153*, **	<0.7	<0.7	1.4	<0.7	<0.7	<0.7	<0.7
PBDE 154*, **	417	155	508	87	354	187	234
PBDE 183**	37	44	0.8	116	55	22	1.1
PBDE 209	296	304	43	190	432	237	99
Polychlorinated alkanes (PCAs)		<i>mg kg⁻¹ d.w.</i>					
SCCP*	1.1	1.5	1.7	0.6	0.9	1.1	2.8
MCCP	2.0	6.6	0.3	1.6	8.8	4.3	3.6
LCCP	30	74	7.9	22	53	45	67
Siloxanes (not included in the PCA model)		<i>µg kg⁻¹ d.w.</i>					
Octamethylcyclotetrasiloxane	280	430	n.m.	n.m.	310	n.m.	n.m.
Decamethylcyclopentasiloxane	22000	19000	n.m.	n.m.	10000	n.m.	n.m.
Dodecamethylcyclohexasiloxane	3100	2600	n.m.	n.m.	2400	n.m.	n.m.
Hexamethyldisiloxane	<2	<2	n.m.	n.m.	<2	n.m.	n.m.
Octamethyltrisiloxane	<2	<2	n.m.	n.m.	<2	n.m.	n.m.
Decamethyltetrasiloxane	16	13	n.m.	n.m.	8	n.m.	n.m.
Dodecamethyltetrasiloxane	46	40	n.m.	n.m.	24	n.m.	n.m.
Terpenes (not included in the PCA model)		<i>µg kg⁻¹ d.w.</i>					
D-limonene	150	n.m.	n.m.	n.m.	n.m.	n.m.	82
L-limonene	350	n.m.	n.m.	n.m.	n.m.	n.m.	70

Fluorinated compounds

Perfluorochemicals (PFCs)	$\mu\text{g kg}^{-1} \text{ d.w.}$						
Perfluorohexane acid (PFHxA)	2.9	<2	2.1	3.0	5.4	<2	<2
Perfluoroheptane acid (PFHpA)	<0.5	<0.5	<0.5	0.62	2.9	<0.5	0.82
Perfluorooctane acid (PFOA)	1.3	0.58	1.3	1.4	10	1.6	0.45
Perfluorononane acid (PFNA)	0.53	<0.4	<0.4	<0.4	14	0.48	<0.4
Perfluorodecane acid (PFDA)	5.9	<0.8	<0.8	<0.8	54	2.5	0.84
Perfluoroundecane acid (PFUnA)	2.2	0.77	<0.6	0.6	112	2.8	<0.6
Perfluorododecane acid (PFDoDA)	4.1	<1.5	<1.5	<1.5	30	3.2	12
Perfluorotridecane acid (PFTrDA)	<1.5	<1.5	<1.5	<1.5	15	<1.5	<1.5
Perfluorotetradecane acid (PFTeDA)	<1.5	<1.5	<1.5	<1.5	2.7	<1.5	<1.5
Perfluorohexane sulfonate (PFHxS)	<0.3	0.36	0.47	1.0	0.47	0.34	<0.3
Perfluorooctane sulfonate (PFOS)**	67	46	6.7	16	30	8.6	12
Perfluorodecane sulfonate (PFDS)	26	5.0	1.5	15	7.5	1.1	0.94
Perfluorooctane sulfonamide (PFOSA)	3.5	0.88	1.2	0.92	5.0	1.5	0.54

Organometals

Organotin compounds (OTCs)	$\mu\text{g kg}^{-1} \text{ d.w.}$						
Monobutyltin (MBT)	228	203	110	202	233	191	106
Dibutyltin (DBT)	234	243	115	263	168	142	116
Tributyltin* (TBT)	9.7	16	5.8	12	12	10	8.3
Monophenyltin (MPhT)	<0.37	<0.37	<0.37	<0.37	<0.37	<0.37	<0.37
Diphenyltin (DPhT)	<0.29	<0.29	<0.29	<0.29	<0.29	<0.29	<0.29
Triphenyltin (TPHT)	<0.43	<0.43	<0.43	<0.43	<0.43	<0.43	<0.43

Metals

	$\text{mg kg}^{-1} \text{ d.w.}$						
As	4.15	3.86	3.75	4.28	3.19	4.58	2.41
Cd*	1.16	1.13	1.18	1.11	0.80	0.78	0.63
Co	9.22	9.96	3.06	7.78	2.84	3.22	6.4
Cr	19.9	24.3	18.6	15.3	28.7	42.4	48.1
Cu	387	433	336	132	337	298	159
Hg*	1.39	0.65	0.39	0.93	1.13	0.66	0.47
Ni*	22.4	17.1	9.89	16.6	9.47	9.92	14.6
Pb*	26.5	29.5	14	17.9	22	27.5	11.7
V	20.4	26.5	17.1	12.4	11.8	25.8	10.1
Zn	501	548	329	569	430	389	252

Pesticides (not included in the PCA model)

Insecticides	$\mu\text{g g}^{-1} \text{ d.w.}$						
Acephate	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
α -cypermethrine	<0.006	<0.006	<0.006	<0.006	<0.006	<0.006	<0.006
Aldrin**	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Azinophosmethyl	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Bromopropylate	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Cyflutrine	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
β -cyflutrine	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Cypermethrine	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
DDD-p,p	<0.06	<0.01	<0.01	<0.05	<0.05	<0.05	<0.01
DDE-p,p	<0.06	<0.01	<0.01	<0.01	<0.01	<0.03	<0.01

DDT-o,p**	<0.05	<0.01	<0.01	<0.05	<0.05	<0.01	<0.01
DDT-p,p**	<0.05	<0.02	<0.02	<0.05	<0.05	<0.06	<0.02
Deltamethrine	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Diazinon	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Dieldrin**	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Dichlorvos	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Dimethoate	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
α -endosulfan*, **	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
β -endosulfan**	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
Endosulfan sulfate	<0.003	<0.003	<0.05	<0.003	<0.003	<0.003	<0.003
Carbaryl	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Carbophenothion	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06
Carbofuran	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Carbosulfan	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Keto-endrin	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
α -chlordane**	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
γ -chlordane**	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002
Chlorfenvinphos*	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
Chlorobenzilate	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Chlorpyrifos*	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
λ -cyhalotrin	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002
Methidathion	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Methoxychlor	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Parathion ethyl	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Parathion methyl	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Permethrine	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Pirimicarb	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Pirimiphos methyl	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Endrin**	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Esfenvalerate	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
Fensulfothion	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Fenvalerate	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Flucythrinate	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3
α -HCH*, **	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
β -HCH*, **	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
δ -HCH*, **	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
γ -HCH (Lindane)*	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004	<0.004
Heptachlor**	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Heptachlorepoxyde	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Propargite	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Propoxur	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Pyridaben	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Quinalphos	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Tetradiphone	<0.09	<0.09	<0.09	<0.09	<0.09	<0.09	<0.09

Herbicides

	$\mu\text{g g}^{-1} \text{d.w.}$						
Glyphosate	0.6	n.d.	<2	0.1	<2	n.q.	0.7
Aminomethylphosphonic acid	5	n.d.	<4	2	10	n.q.	5
Aclonifen	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06
Alachlor*	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Atrazine*	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Desethylatrazine	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.

Desisopropylatrazine	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Cinidon ethyl	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Cyanazine	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Diflufenican	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06
Dichlorobenil	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Diuron*	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Isoproturon*	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Carfentrazone ethyl	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Chloridazon	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Chlorpropham	<0.05	<0.05	<1	<0.05	<0.05	<0.05	<0.05
Metabenzthiazuron	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Metamitron	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3
Methazachlor	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3
Metribuzin	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Pendimethaline	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Ethofumesate	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Phenmedipham	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Flurtamone	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Hexazinone	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Propyzamide	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06
Prosulfocarb	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Simazine*	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Terbutylazine desethyl*	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Terbutryn	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Terbutylazine	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Trifluralin*	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
Fungicides				<i>µg g⁻¹ d.w.</i>			
Azoxystrobin	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
BAM (2,6-dichlorobenzamide)	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Bitertanol	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Cyprodinil	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Diphenylamine	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Captan	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Chlorothalonil	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Quintozene	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Pentachloroaniline	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Metalaxyl	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Prochloraz	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
Fenpropimorph	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Heptachlorobenzene*, **	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002	<0.002
Imazalil	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Iprodione	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Propiconazole	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2
Pyraclostrobin	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Pyrimethanil	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Spiroxamine	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Thiabendazole	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3	<0.3
Tolchlofosmethyl	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03	<0.03
Tolyfluanid	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Vinclozolin	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001

Biocides

	$\mu\text{g kg}^{-1} \text{ d.w.}$						
2-Mercaptobenzothiazole (2MERCAPTOB)	<25	200	<20	250	280	22	950
2-(Tiocyanomethylthio)benzothiazole (2TIOCYANOM)	<50	<50	<50	<50	<50	<50	<50
4-Chloro-3-cresol (KLORKRESOL)	30	19	59	6.8	67	14	<3
N-didecyldimethylammonium chloride (DDMAC)	13000	14000	5600	1400	61000	21000	3000
Propiconazole (PROPICONA)	<2	<5	<5	<0.01	<5	<5	<5
Resorcinol (RESORCINOL)	<10	<25	<50	<10	160	<20	<50
Methylparabene (MEPARAB)	15	52	13	44	59	29	18
Ethylparabene (ETPARAB)	<10	<4	<7	<4	<30	<5	<3
Propylparabene (PROPARAB)	<4	<4	<7	<4	<23	<6	3.6
Butylparabene (BUPARAB)	<4	<4	<7	<4	<23	<5	<3
Benzylparabene (BEPARAB)	<6	<7	<12	<6	<36	<8	<5

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

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