



report

IVL Swedish Environmental Research Institute

Screening tertiary butylphenols, methylphenols, and long-chain alkylphenols in the Swedish environment

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Table of contents

1	Sammanfattning	3
2	Summary	4
3	Introduction	7
4	Tertiary butylphenols	9
4.1	Production and use	9
4.1.1	2,6-di-tert-butyl-4-methylphenol	11
4.1.2	2,6-di-tert-butylphenol	12
4.1.3	4-tert-butylphenol.....	12
4.2	Emission sources	12
4.2.1	2,6-di-tert-butyl-4-methylphenol	12
4.2.2	2,6-di-tert-butylphenol	12
4.2.3	4-tert-butylphenol.....	12
5	Methylphenols.....	14
5.1	Production and use	14
5.2	Emission sources	15
6	Long-chain alkylphenols.....	17
6.1	Production and use	17
6.1.1	Octylphenol.....	17
6.1.2	Nonylphenols	20
6.1.3	Dodecylphenol	20
6.2	Emission sources	21
6.2.1	Octylphenol.....	21
6.2.2	Nonylphenol.....	21
6.2.3	Dodecylphenol	22
7	Toxicity and environmental effects.....	23
7.1	Tert butylphenols.....	23
7.2	Methylphenols.....	24
7.3	Long-chain alkylphenols.....	24
8	Environmental partitioning behaviour and previous measurements	25
8.1	Physical-chemical properties and environmental stability	25
8.2	Environmental partitioning	26
8.3	Previous measurements in the environment.....	29
8.3.1	Tertiary butylphenols	29
8.3.2	Methylphenols.....	29
8.3.3	Long-chain alkylphenols.....	30
9	Sampling strategy and study sites	33
9.1	National	34
9.2	Regional	35
9.2.1	Jönköping.....	35

9.2.2	Värmland.....	35
9.2.3	Skåne.....	36
10	Methods.....	38
10.1	Sampling.....	38
10.1.1	Air sampling.....	38
10.1.2	Sludge sampling.....	38
10.1.3	Sediment sampling.....	38
10.1.4	Water sampling.....	38
10.1.5	Fish samples.....	38
10.2	Analysis.....	39
10.2.1	Chemicals.....	39
10.2.2	Extraction of air samples.....	39
10.2.3	Extraction of sludge and sediment samples.....	40
10.2.4	Extraction of water samples.....	40
10.2.5	Clean up of air, sludge, sediment, and water samples.....	40
10.2.6	Extraction and clean up of fish samples.....	41
10.2.7	Derivatization.....	41
10.2.7.1	Acetylation.....	41
10.2.8	Silica gel chromatography.....	42
10.2.9	GC-MS analysis.....	42
10.2.10	Quality control.....	44
11	Results.....	49
11.1	Tertiary butylphenols.....	56
11.2	Methylphenols.....	57
11.3	Long-chain alkylphenols.....	57
12	Discussion.....	58
12.1	Background regions.....	58
12.1.1	Air.....	58
12.1.2	Fish.....	58
12.1.3	Sediments.....	58
12.2	Municipal sewage treatment plants.....	58
12.2.1	Tertiary butylphenols.....	61
12.2.2	Methylphenols.....	62
12.2.3	Long-chain alkylphenols.....	62
12.3	Point sources.....	63
12.4	Urban environment.....	66
12.4.1	Sediments.....	66
12.4.2	Air.....	66
13	Acknowledgements.....	68
14	References.....	69

1 Sammanfattning

En screeningstudie har utförts med avseende på 30 fenoliska ämnen, däribland 14 tertiära butylfenoler och besläktade substanser, 7 metylfenoler och 9 långkedjiga (C8, C9, C12) alkylfenoler. De huvudsakliga syftena med studien var att bestämma koncentrationer av dessa ämnen i ett flertal olika matriser i den svenska miljön, att spegla viktiga källtyper och att koppla förekomsten i miljön till den nuvarande användningen i Sverige. Ytterligare ett syfte var att undersöka möjligheten för atmosfärisk transport och upptag i biota.

En inventering av användning och möjliga emissionskällor har utförts. Enligt Produktregistret (PR) används 8 av de 14 tertiära butylfenolerna i Sverige, varav 2,6-di-tert-4-metylfenol står för den största använda mängden (ca 270 ton/år). Fyra av de sju metylfenolerna används i Sverige, där 3-metylfenol utgör 98 % av den registrerade konsumtionen (ca 400 ton/år), allt enligt PR. Nonylfenol och dess etoxylater är de långkedjiga alkylfenoler som används mest (ca 230 ton/år), följt av dodekylfenol och små mängder av oktylfenol och dess etoxylater.

Mätningarna utgjordes av ett nationellt samt tre regionala mätprogram om totalt 130 prov fördelade mellan luft, mark, sediment, vatten, avloppsslam och fisk och inkluderade bakgrundsområden, urbana områden, punktkällor och reningsverk. Samtliga studerade ämnen detekterades i slam från reningsverk. Detektionsfrekvensen varierade dock mellan 3% och 100%. Med undantag av enskilda substanser, kan detsamma sägas om sediment och vatten. I luft var metylfenoler den vanligast förekommande ämnesgruppen, medan endast fyra tertiära butylfenoler kunde detekteras och 4-nonylfenol endast i två prov. I fisk detekterades endast två substanser, 4-t-OP och 4-NP, och då bara i ett prov var, vilket indikerar att de undersökta ämnena ej bioackumulerar starkt i fisk.

Tertiära butylfenoler och besläktade ämnen

I slam uppvisade 2,6-di-t-butyl-4-metylfenol, 2,6-di-t-butylfenol, 2,4-di-t-butylfenol och 4-t-butylfenol höga detektionsfrekvenser och relativt höga koncentrationer (i vissa fall > 1 µg/g TS), vilket stämmer väl överens med rapporterad användning. Detta var väntat, då ämnena används i många vanliga hushållsprodukter. Dock återfanns även ett antal ämnen för vilka det inte finns någon rapporterad användning. De fyra dominerande substanserna kunde också detekteras i luft.

Metylfenoler

4-metylfenol dominerade generellt starkt över övriga metylfenoler i slam, sediment och vatten medan koncentrationer i luft var mer likartade för monometylfenolerna. Detta mönster speglar inte den rapporterade användningen. Särskilt anmärkningsvärt är de

höga halterna av 4-MP i ingående vatten till reningsverk (ca 40 µg/l), vilket skulle kunna bero på naturlig nedbrytning av aminosyran tyrosin av tarmbakterier följt av utsöndring med urin. Bakteriell nedbrytning av tyrosin är också en tänkbar förklaring till de höga nivåerna av 4-MP i sediment. Oavsiktlig bildning genom vedförbränning eller atmosfärisk oxidation av toluen och xylen är möjliga källor till metylfenoler i luft.

Långkedjiga alkylfenoler

4-tert-oktylfenol, 4-nonylfenol och dess etoxylater detekterades i de flesta prover av vatten, sediment och slam, och 4-NP var den vanligast förekommande substansen. Dodecylfenol återfanns i färre prover av slam och sediment och aldrig i vatten. 4-t-OP korrelerade starkt med 4-NP i både slam och sediment, vilket indikerar att dessa ämnen har liknande utsläppskällor. Dessutom detekterades de linjära isomererna 4-n-OP och 4-n-NP i låga halter.

Den toxikologiska kunskapen är begränsad för de flesta av de undersökta ämnena, varför det inte är möjligt att göra en kvalitativ bedömning av riskerna med förekomsten av dessa i miljön. Dock kan sägas att koncentrationen av 4-NP överskrider PNEC-värdet i många vattenprover och i de flesta sedimentproverna. Några generella observationer sammanfattas i tabellen nedan. Sammanfattningsvis kan sägas att förekomsten av tertiära butylfenoler och långkedjiga alkylfenoler i miljön speglar användningen i samhället, medan förekomsten av metylfenoler är mer beroende av vedförbränning, oxidation och nedbrytning av andra ämnen.

Ämne	Finns i bakgrundsområden	Anrikas urbant	Vanligt förekommande i slam	Indikationer på industriell påverkan
2,4-di-t-BP			X	x
4-t-BP	XX			x
2,6-di-t-B-4-MP	XX		X	x
2,4,6-tri-t-BP				x
4-MP	XX	X	XX	x
2,3-di-MP	X			x
4-NP		X	XX	x
4-t-OP		X	X	x

2 Summary

A screening study of 30 phenolic compounds is presented, covering 14 tertiary butylphenols and related substances, 7 methylphenols and 9 long-chain (C8, C9, C12)

alkylphenols. The main objectives of the study were to determine environmental concentrations of these substances in a variety of environmental media in Sweden, to highlight important source categories, and to link the environmental occurrence to the current use in Sweden. A further aim was to investigate the likelihood of atmospheric transport and uptake in biota.

An inventory of uses and possible emission sources has been performed. According to the Products Register (PR), 8 out of the 14 tertiary butylphenols are used in Sweden, with 2,6-di-tert-4-methylphenol as the major chemical (ca 270 tonnes/yr). Four of the seven methylphenols are used in Sweden, and 3-methylphenol constitutes 98% of the registered use according to PR (ca 400 tonnes/yr). Nonylphenol and NP-ethoxylates are the major long-chain alkylphenols used (ca 230 tonnes/yr), followed by dodecylphenol and minor amounts of octylphenol and OP-ethoxylates.

The measurements consisted of a national programme and three regional programmes and covered 130 samples distributed between air, soil, sediments, water, sewage sludge and fish, and included background areas, urban areas, near potential point sources, and municipal sewage treatment plants (STP). All chemicals studied were identified in sludge although the detection frequency ranged from 3 % to 100%. Except for single substances, this is also true for sediments and water. In air, methylphenols were the most abundant group, whereas only 4 tertiary butylphenols were detected, and 4-nonylphenol only in two samples. Only two positive identifications were made in fish, 4-t-OP and 4-NP in one sample each, suggesting that these substances do not bioaccumulate strongly in fish.

Tertiary butylphenols and related substances

Abundance in sludge shows a fair agreement with the reported use, with 2,6-di-t-butyl-4-methylphenol, 2,6-di-t-butylphenol, 2,4-di-t-butylphenol and 4-t-butylphenol displaying high detection frequencies and relatively high levels, occasionally exceeding 1 µg/g dw. These substances are the major chemicals used and occur in many household products. However, several substances for which there is no reported use also occur in sludge. The four major chemicals used were also detected in air.

Methylphenols

4-methylphenol generally dominated strongly over the other methylphenols in sludge, sediment and water, whereas levels of individual monomethylphenols were similar in air. This is not in agreement with the reported use. Notable are the high levels of 4-MP in influents to municipal STPs (ca 40 µg/l). It is argued that the origin of 4-MP to STPs is natural, i.e. degradation of tyrosine by intestinal microflora followed by urinary excretion. Bacterial degradation of tyrosine is also a possible explanation for the high levels in sediments. Unintentional formation of methylphenols from wood combustion,

or atmospheric oxidation of toluene and xylene, are possible sources of these compounds in air (e.g., Klotz et al., 1998).

Long-chain alkylphenols

4-tert-octylphenol, 4-nonylphenol and their ethoxylates were detected in most samples of water, sediment and sludge, and 4-nonylphenol was generally the most abundant substance. Dodecylphenol was less frequently detected in sludge and sediments, and never in water. There was a strong correlation between 4-t-OP and 4-NP in both sludge and sediments, suggesting that they are released from similar applications. In addition, low levels of the linear isomers 4-n-OP and 4-n-NP were found.

The toxicological knowledge is very limited for most of these substances, why the risk that these substances pose to the environment rarely can be assessed. The levels of 4-nonylphenol exceed the PNEC-value in many samples of water and in most sediments. Some general observations are summarized in the table below. In conclusion, the environmental occurrence of tertiary butylphenols and long-chain alkylphenols is in fair agreement with the reported use in society, whereas the occurrence of methylphenols appears more strongly influenced by wood combustion, oxidation and degradation processes of other substances.

Substance	Present in background regions	Urban enrichment	High levels and common in sludge	Indications of Industrial impact
2,4-di-t-BP			X	x
4-t-BP	XX			x
2,6-di-t-B-4-MP	XX		X	x
2,4,6-tri-t-BP				x
4-MP	XX	X	XX	x
2,3-di-MP	X			x
4-NP		X	XX	x
4-t-OP		X	X	x

3 Introduction

As an assignment from the Swedish Environmental Protection Agency, IVL has performed a "screening study" of tertiary butylphenols, methylphenols and long-chained alkylphenols. Three county administrative boards have also supplied regional data that are presented in this report. This screening study contains a wide range of substances, all but one including at least one phenol group. The individual substances are summarised together with their CAS-number in Table 1. Alternative names as well as the abbreviations used in this report are also given in the table.

The different substances or groups of substances are emitted to the environment via a variety of sources, including both point sources and diffuse sources such as use in products. They also differ in physical and chemical properties, which affect their transport and distribution in the environment. The physical and chemical properties are summarised in appendix, Table A 19. The occurrence of most of these substances in the Swedish environment is poorly known, as is the importance of different sources.

The main objectives of the study were to determine environmental concentrations of tertiary butylphenols, methylphenols and alkylphenols in a variety of environmental media in the Swedish environment, to highlight important transport pathways, and to assess the possibility and probability of current emissions in Sweden. A further aim was to investigate the likelihood of atmospheric transport and uptake in biota.

A pre-study was carried out in order to identify the major use and emission sources of the selected chemicals (chapter 4-6), which together with the properties of the substances were used to set up a relevant sampling strategy. Measurements have been performed close to possible point sources, in the urban environment (diffuse spreading) and in background areas, covering air, water, soil, sediments, sludge and fish.

Table 1. The compounds included in this study. Group 1: tertiary butylphenols, group 2: methylphenols, group 3: long-chain alkylphenols. i.m.: isomeric mixture.

Group.	CAS	Full Name	Alternative names	Abbreviations used in the report
1	88-18-6	2-tert-Butylphenol		2-t-Butylphenol
1	98-54-4	4-tert-Butylphenol		4-t-Butylphenol
1	2078-54-8	2,6-Diisopropylphenol	Propofol	2,6-Diisopropylphenol
1	1879-09-0	6-tert-Butyl-2,4-xilenol		6-t-Butyl-2,4-xilenol
1	25013-16-5	tert-Butyl-4-hydroxyanisole	BHA	t-Butyl-4-hydroxyanisole
1	96-76-4	2,4-Di-tert-butylphenol		2,4-Di-t-butylphenol
1	97-54-1	Isoeugenol	2-Methoxy-4-(1-propenyl)phenol	Isoeugenol
1	1948-33-0	tert-Butylhydroquinone		t-Butylhydroquinone
1	98-51-1	4-tert-Butyltoluene	TBT	4-t-Butyltoluene
1	128-39-2	2,6-Di-tert-butylphenol		2,6-Di-t-butylphenol
1	52348-51-3	2,6-Di-iso-butylphenol		2,6-Di-iso-butylphenol
1	128-37-0	2,6-Di-tert-butyl-4-methylphenol	Butylhydroxytoluene, BHT	2,6-Di-t-butyl-4-methylphenol
1	4130-42-1	2,6-Di-tert-butyl-4-ethylphenol		2,6-Di-t-butyl-4-ethylphenol
1	732-26-3	2,4,6-Tri-tert-butylphenol		2,4,6-Tri-t-butylphenol
2	95-48-7	2-Methylphenol	o-Cresol	2-Methylphenol
2	108-39-4	3-Methylphenol	m-Cresol	3-Methylphenol
2	106-44-5	4-Methylphenol	p-Cresol	4-Methylphenol
2	105-67-9	2,4-Dimethylphenol	2,4-Xylenol	2,4-Dimethylphenol
2	108-68-9	3,5-Dimethylphenol	3,5-Xylenol	3,5-Dimethylphenol
2	526-75-0	2,3-Dimethylphenol	2,3-Xylenol	2,3-Dimethylphenol
2	95-65-8	3,4-Dimethylphenol	3,4-Xylenol	3,4-Dimethylphenol
3	1806-26-4	4-n-Octylphenol		4-n-OP
3	140-66-9	4-tert-Octylphenol		4-t-OP
3		4-tert-Octylphenol-mono-ethoxylate		4-t-OP-EO1
3		4-tert-Octylphenol-di-ethoxylate		4-t-OP-EO2
3	104-4-5, 25154-52-3	4-n-Nonylphenol		4-n-NP
3	84852-15-3	4-Nonylphenol, branched (i.m.)		4-NP
3	104-35-8	4-Nonylphenol-mono-ethoxylate (i.m.)		4-NP-EO1
3	20427-84-3	4-Nonylphenol-di-ethoxylate (i.m.)		4-NP-EO2
3	27193-86-8	4-Dodecylphenol (i.m.)		4-DP

4 Tertiary butylphenols

Most substances in this group are phenolic compounds, containing at least one tertiary butyl group. Four of the 14 substances are similar to, but are not actually tertiary butylphenols. For ease of presentation, the group will still be referred to as tert butylphenols. The molecular structures and CAS-numbers of the compounds included are shown in Figure 1.

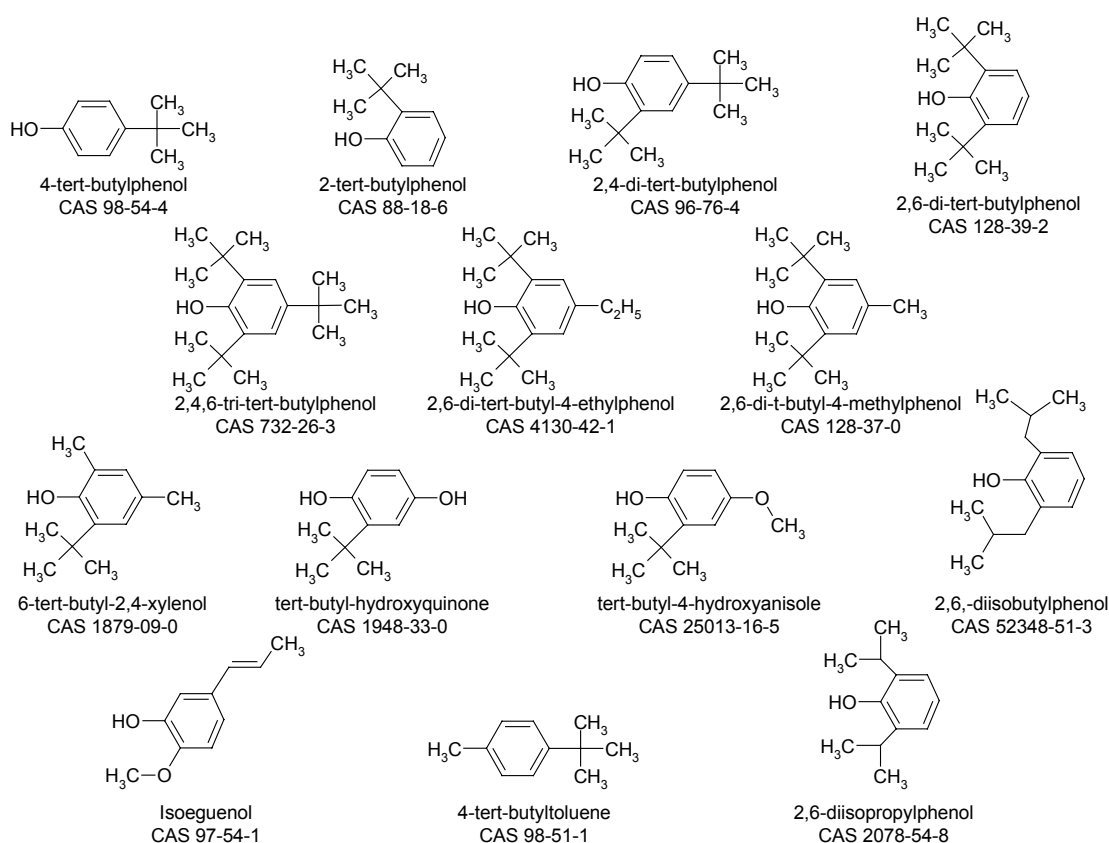


Figure 1. Molecular structures of chemicals belonging to the category “tert butylphenols”.

4.1 Production and use

Tertiary butylphenols are not produced in Sweden, but are imported as pure chemicals and in chemical products. The current use of this substance group in Sweden is about 400 tonnes/year (KEMI, 2003a). The major compounds used are 2,6-di-t-butyl-4-methylphenol and 2,6-di-t-butylphenol, followed by 4-t-butylphenol, t-butyl-hydroquinone and 6-t-butyl-2,4-xenol (Table 2). The total amounts imported each year in the time period 1992-2001 is shown in Figure 2, considering only the import as a pure chemical or chemical product. 2,6-di-t-butyl-4-methylphenol represents more than

50 % of the total use of the substances within the group, in 2001 accounting for 270 tonnes of totally 380 tonnes according to the Product Register (KEMI, 2003a). It is believed that substantial amounts of some of these chemicals are also imported in finished goods.

Use of tertiary butylphenols in Sweden

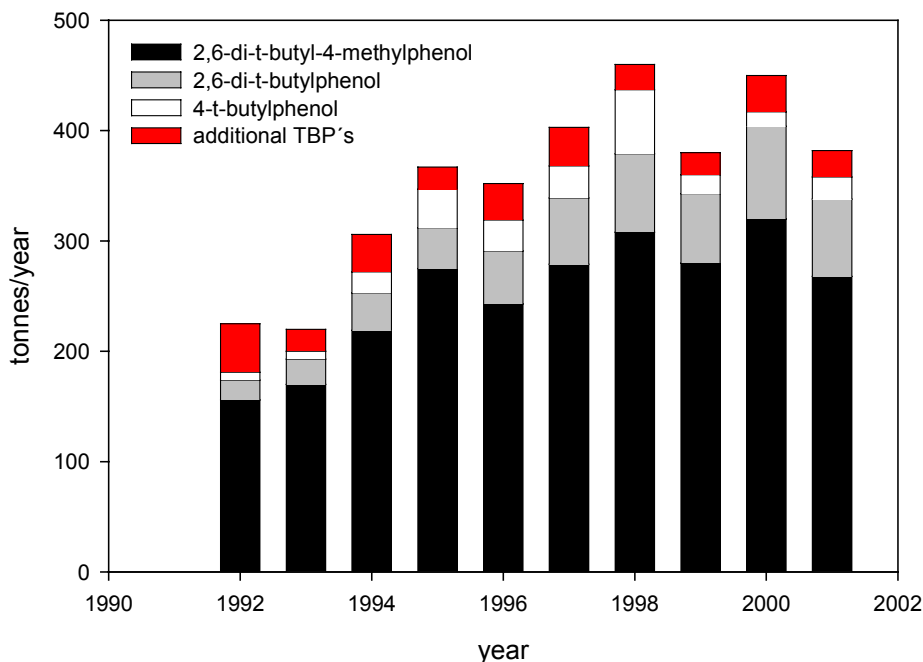


Figure 2. Manufacture and import of the major tertiary butylphenols as pure chemicals or chemical products 1992-2001. Source: Product Register, Swedish Chemicals Inspectorate, Sweden (KEMI, 2003a).

The main products and industries where tertiary butylphenols are used are summarised in Table 2. It should be noted that information about import and/or use is not available for all the compounds in the group. Several compounds are not used in Sweden, according to the Product Register. In some cases, this information is confidential because there is only a limited number of users/importers of that particular chemical.

Table 2. Main products and industries where tert butylphenols are used (KEMI, 2003a; SPIN, 2003).

CAS no	Substance	Use in 2001 (tonnes)	Main products	Main industry
88-18-6	2-t-Butylphenol	1	Lubricant (1999)	Confidential
98-54-4	4-t-Butylphenol	20	Hardener in paints and glue	Paint industry; Building industry
2078-54-8	2,6-Diisopropylphenol	Confidential	Not available/Confidential	Not available/ Confidential
1879-09-0	6-t-Butyl-2,4-xyleneol	0	Not available	Not available
8003-24-5, 25013-16-5	t-Butyl-4-hydroxyanisole	3	Stabiliser	Food industry
96-76-4	2,4-Di-t-butylphenol	4	Lubricant; Stabiliser	Petroleum industry; chemical industry
97-54-1	Isoeugenol	0	Odour agent	Chemical industry
1948-33-0	t-Butylhydroquinone	15	Transmission agent	Rubber and plastic industry
98-51-1	4-t-Butyltoluene	0	Not available	Not available
128-39-2	2,6-Di-t-butylphenol	70	Lubricant; Transmission agent	Petroleum industry; Forest industry; Machinery and Engine workshops
52348-51-3	2,6-Di-iso-butylphenol	0	Not available	Not available
128-37-0	2,6-Di-t-butyl-4-methylphenol	268	Lubricant; Stabiliser; Synthesis raw material; Paints and glue	Rubber ind., Graphical ind.; Metal ind.; Paint ind.; Wood ind.
4130-42-1	2,6-Di-t-butyl-4-ethylphenol	0	Not available	Not available
732-26-3	2,4,6-Tri-t-butylphenol	1	Lubricant (1999)	Confidential

4.1.1 2,6-di-tert-butyl-4-methylphenol

2,6-di-t-butyl-4-methylphenol (also denoted BHT) is the most commonly used chemical within this group (see Table 2) and has a large variety of usage areas, e.g. as an antioxidant, stabiliser, lubricant and as a hardener in rubber, paint, metal, wood, machinery and graphical industry (SPIN, 2003). It is also used as a preservative in groceries and cosmetics (mainly hair styling products, soaps and lotions; SNF 2001, 2004). 2,6-di-t-butyl-4-methylphenol is also a registered antioxidant for food (E320). Since it is not injurious to health, and is added in low levels, there is no obligation to report it to the Product Register. Therefore, the registered use is believed to be underestimated (KEMI, 1998).

4.1.2 2,6-di-tert-butylphenol

2,6-di-t-butylphenol is mainly used as a lubricant and a transmission agent within the petroleum, forestry, machinery and mechanical industry. The registered use has increased over the last 10 years (see Figure 2). In 2001, 2,6-di-t-butylphenol accounted for about 18 % of the total import of the tertiary butylphenols, corresponding to 70 tonnes.

4.1.3 4-tert-butylphenol

4-t-butylphenol is used in construction, paints, plastics (e.g. PVC floors), rubber, and glue industry where its functions are as solvent-based adhesives, hardeners and binders for paint (SPIN, 2003). Phenolic resins containing 4-t-butylphenol are also used for coil coatings within the paint industry (J Fristad pers.comm.). The registered volume used has remained fairly constant since the mid 90s, being about 20 tonnes in 2001.

4.2 Emission sources

Many of the tert butylphenols are expected to be released to municipal wastewater and therefore to the sewage treatment plants (STPs), making the STPs a potential secondary source of emissions. Release to air is also possible for some applications.

4.2.1 2,6-di-tert-butyl-4-methylphenol

2,6-Di-t-butyl-4-methylphenol is supposed to vaporise to air from application of paint, and to indoor air in graphical industries. Food and cosmetics containing 2,6-di-t-butyl-4-methylphenol might be an emission source to municipal STPs. Wastewater from e.g. graphical industries might also contribute to the load of STPs.

4.2.2 2,6-di-tert-butylphenol

2,6-Di-t-butylphenol is an additive in e.g. hydraulic oil. Such spill may thus lead to releases of 2,6-di-t-butylphenol to receiving media, which may be soil or possibly water. Due to lack of detailed knowledge on how and where the oil is applied it is difficult to specify emission pathways.

4.2.3 4-tert-butylphenol

Air is the major media to which 4-t-butylphenol is supposed to be released. Use of glues and solvents containing 4-t-butylphenol contribute to emissions to air, as does application of paint, for example in buildings. Wear of PVC-floors should also be

mentioned but is probably of minor importance. Table 3 summarises the likely emission sources for the compounds in this group in a life-cycle perspective.

Table 3. Possible emissions of tert butylphenols to different media.

	Prod	Industrial use	Private use	Waste	Unintentional
Air	No	Indoor, (graphical industries) Use of solvents, glues etc.	Paint, glues, solvents, wear of PVC-floors	?	No
Water	No	Oil spills		?	No
Soil	No	Oil spills		?	No
STP	No	Wastewater from graphical industries	Through food, cosmetics	?	No

5 Methylphenols

Methylphenols consist of three isomers: 2-methylphenol, 3-methylphenol, and 4-methylphenol (also known as o-cresol, m-cresol and p-cresol respectively). Dimethylphenols are similar, but contain two methyl groups instead of one (Figure 3).

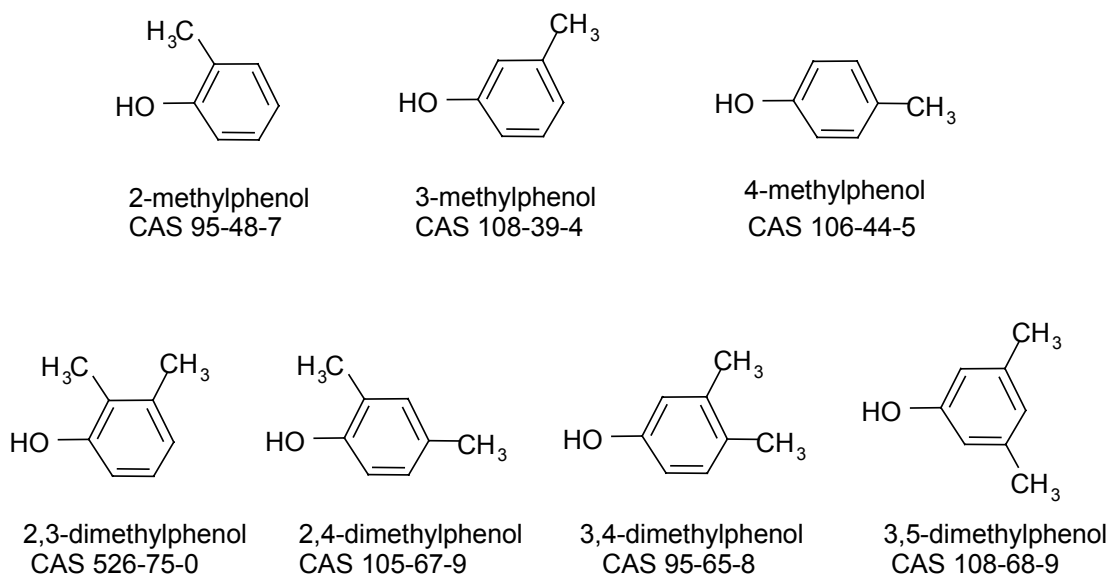


Figure 3. Chemical structures of methylphenols and dimethylphenols.

5.1 Production and use

The major use of the three MPs is as intermediates in the manufacture of chemicals and chemical products (SPIN, 2003 – see Table 4), where 3-methylphenol is the major isomer used. Most of the MPs are extracted from petroleum (KEMI, 1994). Methylphenols are components in coal tar creosote which is mainly used as a wood preservative, but also in pharmacy and smoke flavouring (KEMI, 1994). MPs are constituents also in crude oil (Ioppolo-Armanios, 1996), and they are added to soap as disinfectants, due to their activity as bactericides and fungicides. It has been reported that they are used as antioxidants in some commercial jet fuels to prevent the formation of deposits in aircraft engine fuel systems (ATSDR, 2001). 3-methylphenol, either pure or mixed with 4-methylphenol, has also been important in the production of herbicides (ATSDR, 1992). The use of 3-methylphenol in Sweden has increased from the early 90s to about 400 tonnes in 2001 (Figure 4). Neither the Product Register nor the SPIN database contains any information on the use of dimethylphenols in Sweden.

Table 4. Main products and industries where methylphenols are used.

CAS no	Substance	Use in 2000 (tonnes)	Main product	Main industry
95-48-7	2-methylphenol	2	Not available/Confidential	Chemical industry
108-39-4	3-methylphenol	413	Raw material for chemical synthesis	Chemical industry
106-44-5	4-methylphenol	7	Raw material for chemical synthesis	Chemical industry
526-75-0	2,3-dimethylphenol	Not available	Not available	Not available
105-67-9	2,4-dimethylphenol	Confidential	Not available/Confidential	Not available/Confidential
95-65-8	3,4-dimethylphenol	Not available	Not available	Not available
108-68-9	3,5-dimethylphenol	Not available	Not available	Not available

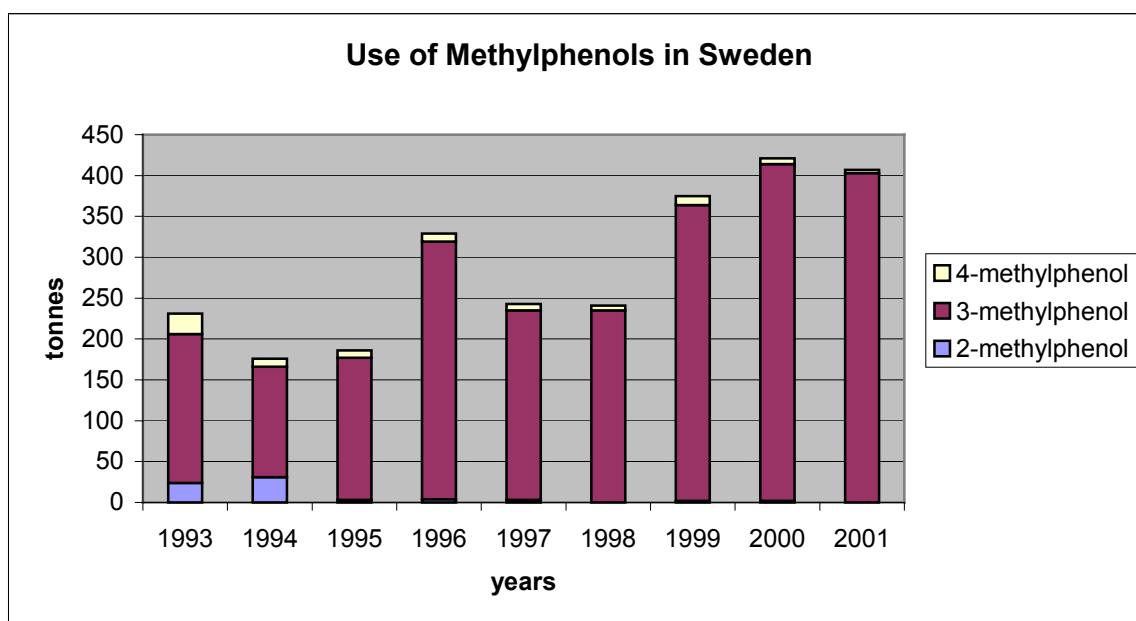


Figure 4. Use of methylphenols in Sweden during the period 1993-2001 (KEMI 2003a).

5.2 Emission sources

The major intentional use of methylphenols is as intermediates in chemical synthesis. Thus, insignificant emissions are expected from private use of chemical products. An exception is creosote, which is only permitted for professional applications. Creosote is used outdoors in sleepers, power lines, enclosures, ports and waterways, where it might be released to the surrounding environment (KEMI, 2004).

In addition to the emissions mentioned above, unintentional releases are also possible. Kurtenbach et al. (2002) suggested emissions of 4-methylphenol directly from road traffic. Emissions of MPs from small-scale biomass burning have recently been estimated (Johansson et al., 2004a). The emission factors of MPs varied significantly between the 20 domestic combustion devices tested. Emissions occurred regardless of the fuel type (pellets or wood), and their magnitude was mainly influenced by combustion conditions together with the type of combustion device. A study in the US also identified emissions of methylphenols from small-scale combustion of wood and these were higher than those of benzene (Schauer et al, 2001). Two orders of magnitude lower emissions were obtained during studies of residential wood combustion (McDonald et al., 2000).

Both methylphenols and dimethylphenols may also be subject to secondary formation in the atmosphere, through reactions between hydroxyl radicals and toluene or xylene respectively (e.g. Klotz et al., 1998). Methylphenols may also be formed through biodegradation of toluene (Neilson, 2000). Thus all sources of toluene and xylene, e.g. gasoline, are potential sources also of methyl- and dimethylphenols. A summary of possible emission sources are given in Table 5.

Table 5. Possible emissions of methylphenols to different media.

	Industrial prod	Industrial use	Private use	Unintentional emission
Air	yes	Wood preservatives (creosote); coal tar refining; metal refining	Paint?	Road traffic; Wood combustion;
Water	yes	Leaching from creosote	Paint?	Storm water from road traffic
Soil	?	Leaching from creosote treated wood	Creosote treated sleepers	
STP		Soap, wood pulping		

6 Long-chain alkylphenols

The group of chemicals here referred to as “long-chain alkylphenols”, contains octyl- and nonylphenols and their ethoxylates, and p-dodecylphenol. Long-chain alkylphenols are characterised by having either a straight alkyl chain or a branched alkyl group connected to the phenol. Their names depend on where on the phenol the alkyl group(s) is situated, the length and branching of the alkyl chain. The nomenclature of nonylphenols is somewhat inconsistent. According to the Swedish National Chemicals Inspectorate (E. Ljung, pers. comm.), the following is correct:

- ✓ 104-40-5: straight nonylchain in para position
- ✓ 25154-52-3: straight nonylchain, but not necessarily in para position
- ✓ 84852-15-3: branched nonylchain in para position, probably the major isomer used.

According to ECB (2002), CAS-no 25154-52-3 previously included all ”nonylphenols”, but has been redefined to only contain the nonylphenol with a straight alkylchain, and others have been assigned new CAS-nos. The term “nonylphenol” is, however, still used as a general term for all nonylphenols. Also dodecylphenols are registered under several CAS-numbers, and there appears to be confusion regarding which isomers that correspond to different CAS-numbers. The long-chain alkylphenols investigated in this study are shown in Figure 5.

6.1 Production and use

The principle products commercially available are ethoxylates of para-octylphenol (once the major product), para-nonylphenol, dinonylphenol (mixture of isomers) and para-dodecylphenol. The ethoxylate chain length in these products are much longer than 1 or 2, i.e. the ethoxylates analysed are degradation products. The most common alkylphenol ethoxylates are the nonylphenol ethoxylates, which are made using distilled nonylphenol (usually >90% para). The nonylphenol group is derived from a propylene trimer and therefore the alkyl group is a branched chain (Porter, 1994). Table 6 summarises the main uses of long-chain alkylphenols and their ethoxylates in Sweden in 1999 and 2000 (SPIN, 2003).

6.1.1 Octylphenol

There is currently very limited information on the Swedish use of octylphenol and octylphenol ethoxylates. Globally, the use of octylphenol generally follows the pattern shown in Figure 6. Additionally, it has been reported that octylphenol is present as an

impurity (3-5%) in commercial grade nonylphenol (OSPAR Commission, 2003). However, by considering the method by which the nonylchain in NP is synthesized (from propylene units), octylphenol should not be expected as an impurity. Analysis of technical nonylphenol at the IVL laboratory showed that 4-t-OP was <0.004 % in this product, i.e. in contradiction with the statement in the OSPAR report.

The European net use of octylphenols increased from 18 000 tonnes in 1997 to almost 23 000 tonnes in 2001 (OSPAR Commission, 2003). It is reasonable to believe that at least a few percent of this volume reaches Sweden, in which case the figures in Table 6 can be regarded as an underestimate.

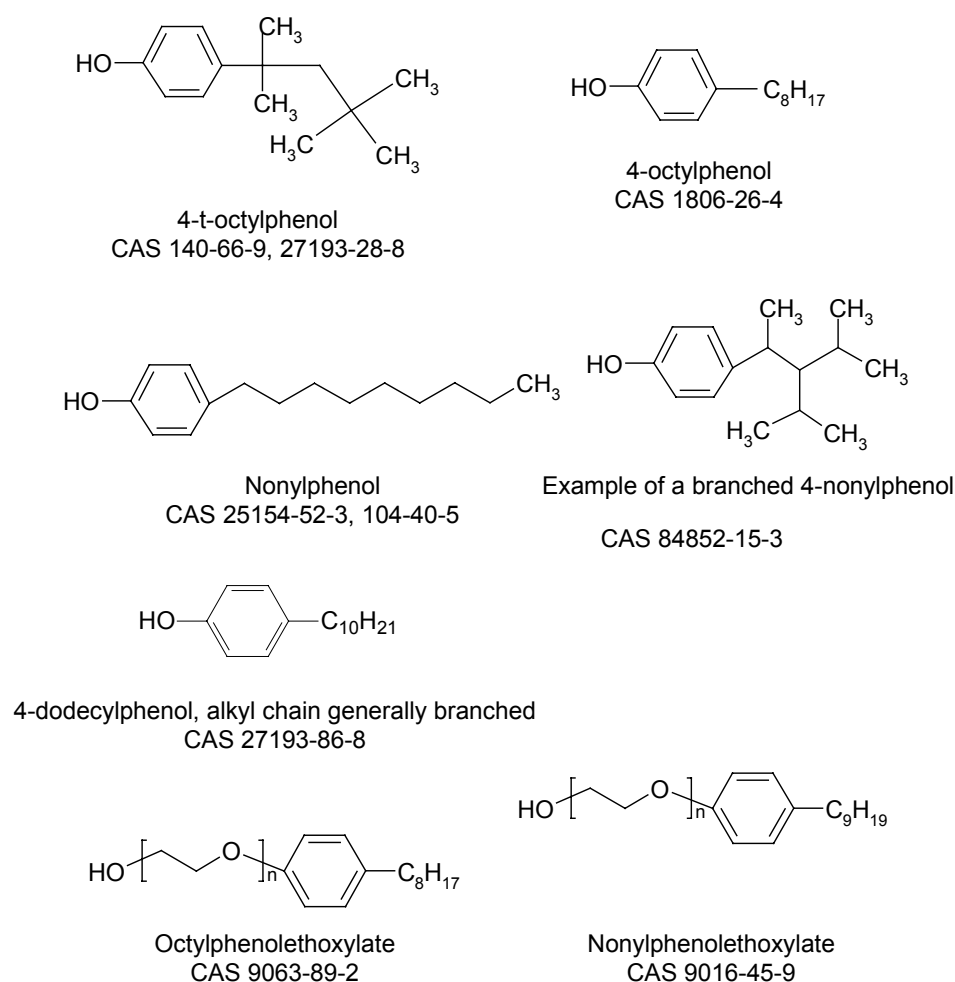


Figure 5. Structures of long-chain alkylphenols and their ethoxylates.

Table 6. Major uses of long-chained alkylphenols and alkylphenol ethoxylates in Sweden (SPIN, 2003).

CAS no	Substance	Main product	Main industry	1999 (tonnes)	2000 (tonnes)
1806-26-4	p-octylphenol			-	-
140-66-9	p-tert-octylphenol	Raw material for chemical synthesis	Rubber and plastics industry	8	6
9063-89-2	Octylphenol-ethoxylates	Not available/ Confidential	Rubber and plastics industry	1	1
25154-52-3	Nonylphenol ^A	Hardener in plastics and paint	Construction and plastics industry	19	36
104-40-5	4-Nonylphenols ^A	Raw material for chemical synthesis	Chemical industry	15	29
84852-15-3	4-nonylphenol, branched	Not available	Not available	21	1
127087-87-0	Nonylphenol, branched			0	0
9016-45-9	Nonylphenol-ethoxylates	Paints, glue, emulsifier	Paint stores, building-, paper-, paint-, textile industry	142	173
27193-86-8	p-Dodecyl-phenol	Lubricant	Coke and petroleum, Wholesale and retail	96	75

^A It is possible that these amounts are registered under the wrong CAS-no, and that it actually is the branched isomer that is used (84852-15-3).

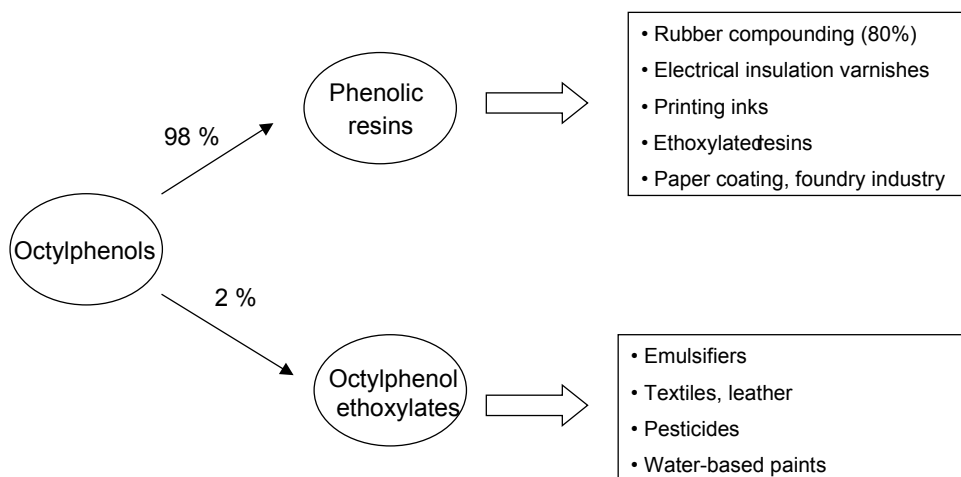


Figure 6. The international use of octylphenol according to OSPAR Commission (2003)

6.1.2 Nonylphenols

The Swedish production of nonylphenols has recently ceased but import as raw material still occurs. The current use of nonylphenols and their ethoxylates (NPEs) is illustrated in Figure 7.

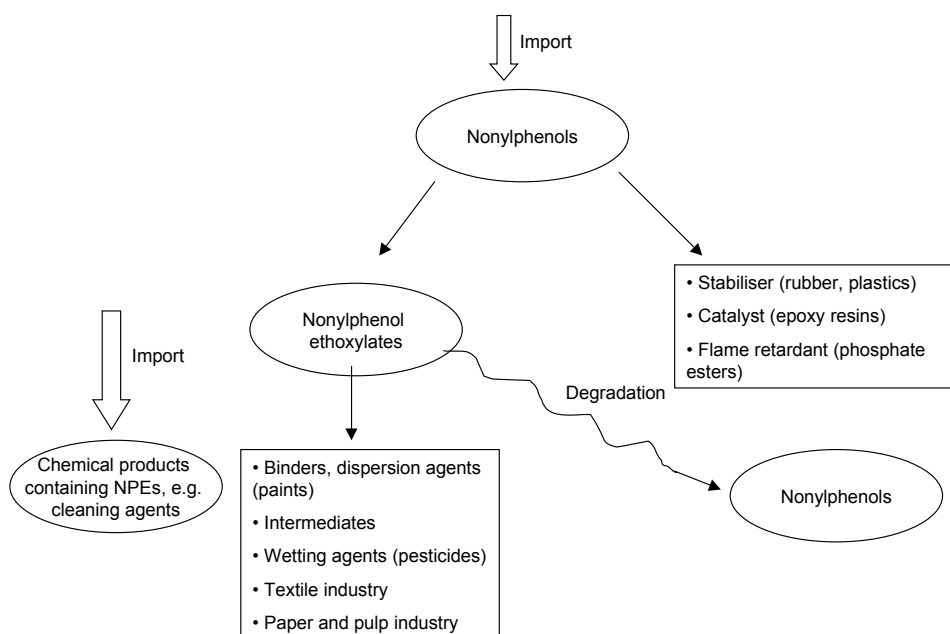


Figure 7. Current use of nonylphenols and their ethoxylates in Sweden (Krook, 2004; Ferguson and Brownawell, 2003; KEMI, 2001; SPIN, 2003; ECB, 2002).

Previously, NPEs were used in larger quantities and in a larger variety of chemical products (e.g. tensides in cleaning agents, viscosity decreasing agent in PVC-floor production, surfactants, lubricants, cutting and drilling fluids; KEMI, 2001), but the use decreased more than 90 % during the 1990s (3000 tonnes in 1990; KEMI, 2001). This decrease was partly due to voluntary phase-out of NPEs in cleaning agents within the EU. As evident from Figure 7, import in such products may still be possible from other countries. As shown in the figure, the NPEs can also degrade to nonylphenols in the environment (Ferguson and Brownawell 2003).

6.1.3 Dodecylphenol

There is no production of dodecylphenol in Sweden, but import in chemical products. Internationally, dodecylphenol is primarily used as intermediate in the production of oil and lubricant additives (99 % of use; Watts & Mitchell, 2003), and import of such products to Sweden occurs (KEMI, 2003b).

6.2 Emission sources

As there is no production of long-chain alkylphenols in Sweden, the releases to the environment are more likely to come from the processing industry and from private and professional use of certain products. In the following subchapters, possible emission scenarios are presented, considering the use described above. Although emissions are considered in a life-cycle perspective, the waste stage is not explicitly discussed. In principle the four major alternatives are:

- ✓ Landfills – release to water over long time; possibly emissions to air
- ✓ Incineration – alkylphenols should be destroyed during combustion
- ✓ Recycling – emissions depend on actual process
- ✓ Sewage treatment plants – industrial wastewater may be treated on site before discharge to municipal STP or recipient. It is likely that households contribute with octyl- and nonylphenols to STPs. It is widely recognised that octyl- and nonylphenols are released via sewage treatment plants. Octyl- and nonylphenol ethoxylates are degraded to octyl- and nonylphenols in STPs.

6.2.1 Octylphenol

Due to the lack of detailed information on the Swedish use of octylphenols and their ethoxylates (see discussion in chapter 6.1.1), it is not possible to produce a qualitative emission assessment. Briefly, emissions do likely occur as a result of certain industrial activities and/or waste disposal. The occurrence of octylphenol in chemical products and goods used in household is poorly known, why the likelihood of diffuse emissions cannot be estimated.

6.2.2 Nonylphenol

As mentioned in chapter 6.1.2, NPEs occur in a variety of household products, such as water-based paints, which are likely to end up in municipal STPs. Due to degradation of NPEs to nonylphenols, STPs have traditionally been considered as major emission sources of these chemicals. Recent environmental monitoring suggests that also diffuse emissions are important (Sternbeck et al., 2003). NPEs may e.g. vaporise to air during application of water-based paints on house facades, which may result in higher atmospheric emissions of NPEs in residential areas. Process water from textile and paper & pulp industries are likely to be discarded to the STP, even though many industries have their own wastewater treatment. NPEs may be emitted to soil and to the wastewater system through spills and leaks of oils, mainly during industrial use. Table 7 summarises the possible emission pathways of nonylphenols in a life-cycle perspective.

Table 7. Possible emissions of nonylphenols.

	Ind prod	Industrial use	Private use
Air	No		Paint vaporisation from house facades
Water	No	Oil spills and leaks	Water runoff from painted houses,
Soil	No	Oil spills and leaks	Use of pesticides
STP	No	Cleaning products, paper- & pulp industry drainage, drainage from textile industries	Use of imported cleaning products containing NPEs

6.2.3 Dodecylphenol

As discussed in chapter 6.1.3, the use of dodecylphenol is fairly limited in Sweden, why emissions of this compound is expected to be low. The most likely source for environmental releases in Sweden is spills and leakage of oils and fuels containing dodecylphenols, mainly resulting from industrial activities (Table 8).

Table 8. Possible emissions of dodecylphenols.

	Industrial prod.	Industrial use	Private use
Air	No	No	No
Water	No	Oil and fuel spills and leakage	No
Soil	No	Oil and fuel spills and leakage	No
STP	No	No	No

7 Toxicity and environmental effects

This section compiles information on toxicity of the chemicals studied. Information on classification for health and environment was taken from www.kemi.se. Examples of PNEC values (predicted no effect concentration) derived for the alkylphenols are given in Table 9. It must be emphasised that the confidence to individual PNEC values depends on the number and quality of studies from which they are derived. The assessment factor (AF) reflects this uncertainty. A high AF indicates that only a few toxicity studies have been performed, sometimes only using one single species, whereas a lower assessment factor accounts for a more thorough existing knowledge on the chemical's toxicity. Therefore, a low PNEC value does not necessarily imply a very toxic chemical, but can also be a result of poor understanding of the toxicity. The PNEC value for sediments was estimated from the corresponding value for water, assuming equilibrium partitioning (see TGD, 2002, for a discussion of inherent uncertainties).

Table 9. Effect scoring for organic substances in the aquatic phase (Klein et al., 1999).

CASno	Substance	Endpoint ^a	Conc (µg/l)	AF	PNEC _{water} (µg/l)	PNEC _{sed} (µg/kg)	Ref
98-54-4	4-t-butylphenol	LC50f	1600	1000	1.6		Klein et al., 1999
98-51-1	4-t-butyltoluene	NOECa	5600	100	56		Klein et al., 1999
95-48-7	2-methylphenol	LC50f	2000	1000	2		Klein et al., 1999
108-39-4	3-methylphenol	LC50f	6000	1000	6		Klein et al., 1999
106-44-5	4-methylphenol	NOECa	11000	100	110		Klein et al., 1999
140-66-9	4-t-octylphenol	NOECf	6.1	10	0.61		Klein et al., 1999
25154-52-3	Nonylphenol	NOECc	3.3	10	0.33	39	(ECB, 2002)

^a f – fish, a – algae c – crustacean

7.1 Tert butylphenols

None of tert butylphenols or their associated substances are classified for health or environment in Sweden. According to OECD (1995), 2,6-di-tertbutylphenol is very toxic for water organisms and is not biodegradable. The lowest acute toxicity was reported for daphnids (EC50 48h = 0.45 mg/l). For humans, the substance is not acutely toxic, but irritant to skin and eyes. 4-tert-butylphenol is considered to be an irritant to

the skin, eyes, and respiratory tract (OECD, 2000). Table 10 summarises the results of various toxicity studies concerning t-butylphenols.

Table 10. Toxicity of some butylphenols.

CASno	Substance	Endpoint	Conc (µg/l)	Ref
128-39-2	2,6-di-tertbutylphenol	NOELc (96h)	380	OECD, 1995
128-39-2	2,6-di-tertbutylphenol	NOECc	76	OECD, 1995
128-39-2	2,6-di-tertbutylphenol	NOELf	<210	OECD, 1995
128-39-2	2,6-di-tertbutylphenol	NOELf	300	OECD, 1995
98-54-4	4-t-butylphenol	NOECa	9530	OECD, 2000
98-54-4	4-t-butylphenol	NOECc	730	OECD, 2000
98-54-4	4-t-butylphenol	LC50f	5100	OECD, 2000

7.2 Methylphenols

Methylphenols and 3,5-dimethylphenol are classified as toxic through skin contact and during consumption. Furthermore, the three dimethylphenol isomers are also toxic to water-living organisms and may cause long-time effects in the environment (KEMI, 1994).

7.3 Long-chain alkylphenols

Nonylphenol is classified as injurious to health, hazardous during consumption and corrosive, and is also classified as harmful to the environment and very toxic to aquatic organisms. Dodecylphenol meets the criteria for a PBT (Persistent, Bioaccumulative, Toxic) chemical (Watts & Mitchell, 2003). Nonylphenol and nonylphenol ethoxylates have been found to exert estrogenic effects in aquatic organisms (ECB, 2002).

The log K_{ow} for dodecylphenol implies a moderate to high bioaccumulation potential in aquatic biota, which is supported by a measured bioconcentration factor (BCF) value of 6000 for fish and an estimated BCF of about 9000 (Watts & Mitchell, 2003).

8 Environmental partitioning behaviour and previous measurements

The chemicals described in previous chapters have varying physical-chemical properties, and thus different partitioning properties. In order to investigate the partitioning behaviour of the chemicals, and thereby predict the likely receiving media, a modelling exercise was performed, using the generic steady-state multimedia fugacity model known as the “Equilibrium Criterion Model” (EQC; Mackay et al., 1996). The outcome of this exercise was intended to serve as support to the set-up of the sampling programme.

The EQC model describes a generic environment, consisting of four compartments: air, water, soil and sediment in an area of a size equal to that of the Netherlands. Physical-chemical property data were compiled for all the substances (see Appendix, Table A 19) and two different emission scenarios were considered, based on the information obtained in chapters 4-6. The scenarios considered were a) simultaneous emissions to all media (air, soil and water), representing cases of e.g. oil leakage and spills and b) emission to water only, representing e.g. emissions from sewage treatment plants or emissions to storm water. In all cases, the emission rate was 1000 kg/h. This is of course highly overestimated, but as the model is linear, and the assessment was used for comparative reasons, the absolute values have no influence on the outcome.

8.1 Physical-chemical properties and environmental stability

The physical-chemical properties used in the modelling exercise are listed in Appendix, Table A 19, median values and ranges being shown in Table 11. All chemicals in the three groups are considered to be reactive in the atmosphere with relatively short half-lives (<20h; see Appendix, Table A 19), thus the occurrence in air is expected to be low. The t-butylphenols may oxidise and re-reduce in the atmosphere, but only one of them, t-butylhydroquinone may alternate between its oxidised and reduced form (Lopez-Avila and Hites 1981; Oros and David 2002). The others form different compounds when re-reduced. Atmospheric oxidation is expected also for methylphenols ($t_{1/2} \approx$ one day; OECD, 2000) and the nonylphenols have been reported to be reactive with hydroxyl radicals (ECB, 2002). Therefore, atmospheric long-range transport is unlikely for the chemicals investigated.

The tertiary butylphenols display a varying degradation pattern under aerobic conditions. 4-t-butylphenol has been reported to be readily biodegradable, whereas 2,6-di-t-butylphenol biodegrade poorly (OECD, 2000). Some photodegradation is expected

for both compounds (OECD, 2000). Methylphenols have been reported to be readily biodegradable under aerobic conditions, with $t_{1/2} \approx$ one day-one week in water (ATSDR, 1992), and rapid degradation has also been observed under anaerobic conditions (e.g. Heider & Fuchs, 1997; Spence et al., 2001). Nonylphenols on the other hand, have shown to be stable under anaerobic conditions (Hesselsøe et al., 2001). Nonylphenolethoxylates have been observed to degrade under anaerobic conditions in digested sewage sludge, forming nonylphenols, which remained stable (e.g. Ejlertson et al., 1999).

Appendix, Table A 19 lists estimated half-lives in air, water, soil and sediment. These half-lives are based on the estimation software known as EPIWIN (Meylan, 1999). It should be noted that these values are associated with large uncertainties, but as no consistent data sets on degradation in various media exists for all these chemicals, it was decided to use the same data source for all the compounds for the modelling exercise.

Table 11. Physical-chemical properties of substances in the three groups. Median values are shown, with total range in brackets.

Property	Tert butylphenols	Methylphenols	Long-chain alkylphenols ^A
MW	192 (148-361)	122 (108-122)	220 (206-262)
Solubility in water, mg/l	35 (0.6-750)	7 900 (4 600-26 000)	5 (0.03-7)
Vapour pressure, Pa	0.66 (0.03-89)	14 (4.7-39)	0.013 (0.0003-0.06)
LogKow	4.7 (2.9-6.1)	2.2 (1.95-2.5)	5.6 (5.3-6.6)

A. Data include the ethoxylates.

8.2 Environmental partitioning

Figure 8 and Figure 9 show the predicted percentage distribution between air, water, soil and sediment considering the two emission scenarios presented above. The major goal of this exercise is to compare the expected environmental partitioning between the groups. The absolute percentage values must not be interpreted to exactly; it is the trend between the chemicals that is of interest.

As shown in the figures, the EQC model predicts only minor amounts of all chemicals to partition to air regardless of emission scenario. This is consistent with the discussion above concerning atmospheric stability and potential for long-range transport. When emitted to all media (Figure 8), the t-butylphenols and the long-chain alkylphenols are distributed between water, soil and sediment with the majority partitioning to soil and

sediment (t-butylphenols mainly to soil), whereas the methylphenols are predicted to mainly partition to water and soil.

When emitted only to water, all chemicals are predicted to be distributed between water and sediment with the exceptions of methylphenols, which all partition to water. The partitioning behaviour is generally much more heterogeneous for t-butylphenols than for long-chain alkylphenols, the latter showing a clear preference of sediment compared to water.

The partitioning behaviour is dependent on the medium of release, mainly in terms of percentage partitioning to soil, thus the emission pathways are important factors when deciding which matrices that should be sampled.

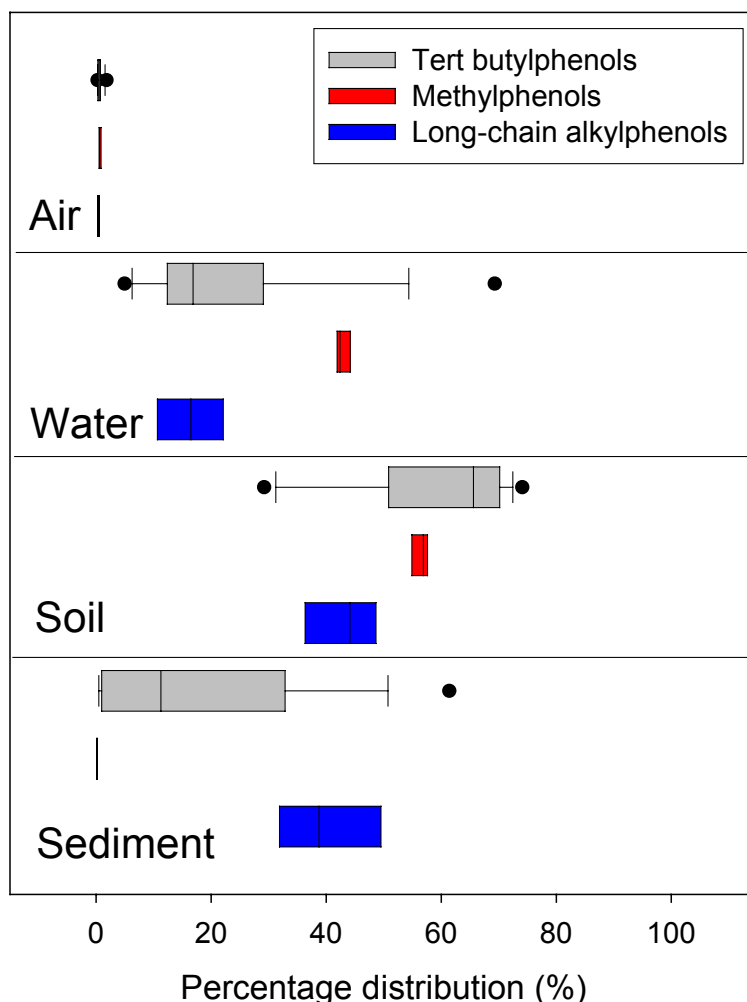


Figure 8. Predicted environmental partitioning considering parallel emissions to air, water and soil.

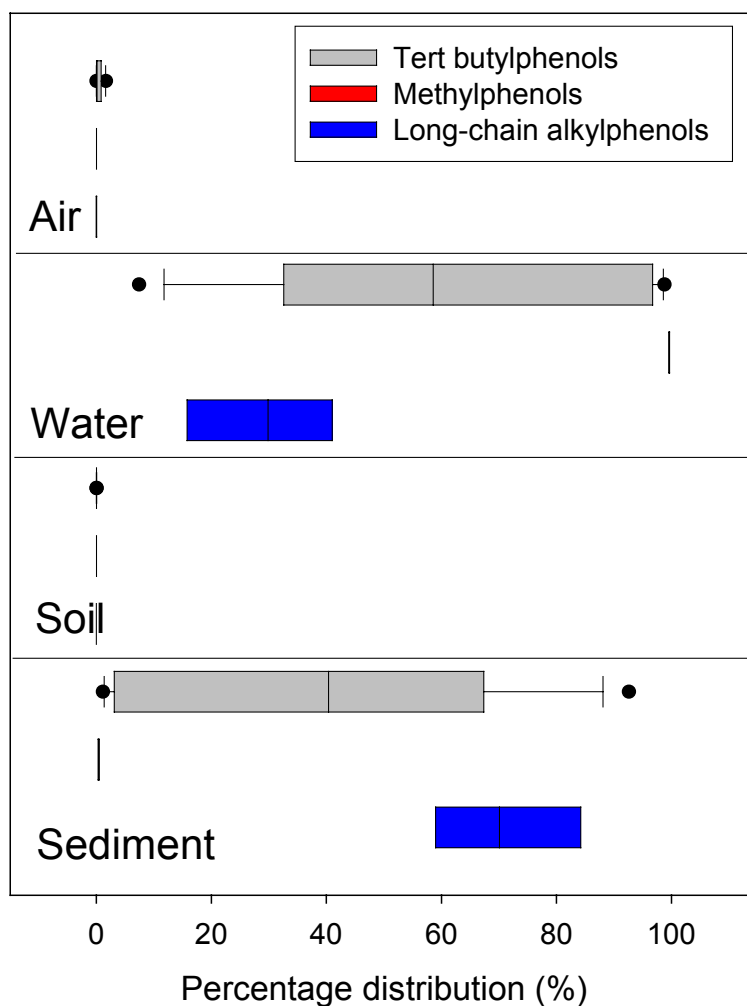


Figure 9. Predicted environmental partitioning considering emissions to water only

The modelling results support the hypothesis that the atmospheric compartment is of low importance for the occurrence and transport of these compounds in the environment and that the main transport pathway should be via aquatic systems. The small amounts present in the air can, however, be enough to allow for transport if the chemical lifetime is long enough. This has proven to be the case for many other hydrophobic, low-volatile chemicals such as e.g. PCBs and PBDEs.

8.3 Previous measurements in the environment

8.3.1 Tertiary butylphenols

Data on the environmental occurrence of tert butylphenols are scarce. The most commonly reported substance is 2,6-di-t-butyl-4-methylphenol, which previously has been detected in Swedish influents and effluents from STPs. Between 70-100 % was estimated to derive from households (Paxeus, 1999). 2,6-Di-t-butyl-4-methylphenol has also been reported to occur in Dutch STP effluents (concentration unknown; van Wezel & Kalf, 2000) and in US rivers. A compilation of data is given in Table 12.

Table 12. Previous environmental measurements of tert butylphenols.

Media	Study area	Concentrations	median	det.freq. (%)	Reference
2,6-Di-t-butyl-4-methylphenol (BHT)					
Incoming wastewaters	Sweden	14-42 µg/l			Paxeus, 1999
STP effluents	Sweden	1.2-24 µg/l			Paxeus, 1999
river water, downstream societies	USA	max 0.1 µg/l	0.1 µg/l	2.4	Kolpin et al., 2002
2,6-Di-t-butylphenol					
Incoming wastewaters	Sweden	25-145 µg/l			Paxeus, 1999
STP effluents	Sweden	1.8-21 µg/l			Paxeus, 1999
river water, downstream societies	USA	max 0.11 µg/l	0.06 µg/l	3.5	Kolpin et al., 2002
t-butyl-4-hydroxyanisole					
Incoming wastewaters	Sweden	0.2-0.5 µg/l			Paxeus, 1999
river water, downstream societies	USA	max 0.2 µg/l	0.1 µg/l	2.4	Kolpin et al., 2002

8.3.2 Methylphenols

Methylphenols have recently been measured in air in two Swedish cities during wintertime, Lycksele in the north and Växjö in the south (Johansson et al., 2004b, c). The average concentrations for the sampling periods are given in Table 13.

Table 13. Atmospheric levels of methylphenols in two Swedish cities.

	Average ng/m ³	median ng/m ³	min ng/m ³	max ng/m ³	Number
Lycksele Jan-Mar 2002					
Sampling station strongly influenced by domestic biomass burning					
2-methylphenol	7.4	4.0	1.3	23	15
3-methylphenol	4.2	2.7	0.5	18	15
4-methylphenol	9.0	5.2	0.6	46	15
Sampling station influenced by domestic biomass burning					
2-methylphenol	10	12	1.2	25	15
3-methylphenol	5.6	5.6	1.3	12	15
4-methylphenol	14	13	2.4	33	15
Växjö Jan-Mar 2002					
City Center					
2-methylphenol	13	5	1.8	41	14
3-methylphenol	4.2	2.5	<1	16	14
4-methylphenol	11	4.7	<1	41	14
Sampling station influenced by domestic biomass burning					
2-methylphenol	11	8	1.7	29	14
3-methylphenol	4.6	3.4	0.6	12	14
4-methylphenol	12	10	<1	37	14

8.3.3 Long-chain alkylphenols

Alkylphenols and their ethoxylates have been found in fish and in storm water, landfill leachate and ground water at different sites in Sweden (Table 14 and Table 15). Octylphenols and nonylphenols have also been detected in sewage sludge and sediment in Stockholm and the Svealand coastal region (Table 16 and Table 17). Levels of nonylphenol in municipal sewage sludge from Stockholm decreased strongly during the early 1990s, as a result of more restricted use of certain products. Concentrations were close to 1000 mg/kg dw during 1990 and present annual averages are 23-30 mg/kg dw (C. Wahlberg, pers. comm.).

Table 14. Previous measurements of octylphenols and nonylphenols in Swedish biota.

Substance	Media	Content in biota	no of samples	Reference
4-t-OP	Fish	<18 - 350 ng/g fat	21	Öberg et al, 2003
NP	Mussels	200-400* ng/g fresh weight	1	Wahlberg et al 1999 ; levels may influenced by point source.

Table 15. Previous measurements of octylphenols and nonylphenols in water in Sweden (µg/L)

	Storm water	Sewage water i=incoming, e=effluent	Landfill leachate	Groundwater	Recipient water
4-t-OP	0.06-0.7 (n=3)	0.3-1.7 i 0.1-0.7e	0.3, 10 (n=2)	0.06	0.04
4-t-OP-EO1	0.2-1.4 (n=3)	0.1-2.6 i <0.1-0.4 e	0.04-0.2 (n=3)	0.05	0.06
4-t-OP-EO2	0.7 (n=2)	0.1-1.2 i <0.1-0.6 e		0.2	
4-NP	0.2-0.8 (n=3)	0.6-36.9 i 0.4-17.7 e	1.5-4.1 (n=3)	2.5	0.2
4-NP-EO1	0.2-14 (n=3)	<0.1-15 i 0.1-4.7 e	5.4-6.0 (n=3)	0.2-0.4	
4-NP-EO2	0.3-10 (n=3)	0.6-12.3 i <0.1-6.0 e	0.7	0.5	
Reference	Junestedt et al., 2003	Paxeus, 1999	Junestedt et al., 2003	Junestedt et al., 2003	Junestedt et al., 2003

Table 16. Previous measurements of octylphenols and nonylphenols in sewage sludge.

Substance	STPs	Conc. (µg/g dw)	no of samples	Reference
4-t-OP	Stockholm	0.78-0.96	2	Sternbeck et al, 2003
4-NP	National average, 1995	46.6	ca 400	SCB, 2004
4-NP	National average, 1998	22.8	ca 400	SCB, 2004
4-NP	National average, 2002	17.2	ca 400	SCB, 2004
4-NP	Stockholm	31-44	2	Sternbeck et al, 2003

Table 17. Previous measurements of octylphenols and nonylphenols in sediment in Sweden.

Substance	Study area	Conc. range (ng/g dw)	median (ng/g w)	no of samples	Reference
4-t-OP	Suburban lakes, Stockholm	2-140	15	13	Sternbeck et al, 2003
4-t-OP	Central Stockholm	0.3-7.6	4.4	7	Sternbeck et al, 2003
4-t-OP	Baltic coast	<1-9.1	ca 1.5	14	Sternbeck et al, 2003
4-NP	Suburban lakes, Stockholm	67-5300	1500	13	Sternbeck et al, 2003
4-NP	Central Stockholm	12-510	310	7	Sternbeck et al, 2003
4-NP	Baltic coast	<20-380	ca 45	14	Sternbeck et al, 2003

9 Sampling strategy and study sites

This screening study consists of a national programme and separate regional programmes for three counties (Figure 10). The sampling strategies are described below and an overview is given in Table 18.



Figure 10. Map of Sweden with the three counties and Stockholm marked.

Table 18. Number of samples per media, in the national and regional programmes, respectively.

Media	National	Jönköping	Skåne	Värmland	Total
Incoming waste water to STP		4	5	1	10
STP effluent	13	4			17
Storm water		3	5		8
Fish	3		10		13
Air	19				19
Soil	3				3
Lake water			1		1
Sediment	17	4	1	5	27
Sewage sludge	12	4	10	3	29
Surface water	2			1	3
Total	69	19	32	10	130

9.1 National

Many of the chemicals investigated are used in mechanical/technical industry. They also occur in a variety of household products, and are therefore likely to become dispersed and distributed throughout the society, and possibly accumulate in densely populated areas. Emissions may thus occur both from point sources and by diffuse pathways from society, including sewage systems (chapters 4, 5 and 6). The national sampling programme is summarised in Table 19.

Several samples were taken in triplicate, in order to illustrate the natural variation of concentrations within a certain sampling matrix. These samples were taken closely in time, and do thus not illustrate seasonal changes in e.g. sewage treatment plants.

Table 19. Selected sites in the national programme.

Site	Details	Air	Water	Soil	Sediment	Sludge	Fish
Background							
Råö		X					
Fladen							X
Pallas		X					
Urban							
Stockholm		X			X		
Malmö		X					
Industrial source							
Anonymous Paint industry	Possible use of long-chain alkyl- and butylphenols	X	X		X	X	
Trollhättan	Industrial area	X		X			
Perstorp	Chemical industry, phenolic resin producer	X	X		X	X	
Stenungsund	Chemical/plastics industry, previous detection of alkylphenols	X			X	X	
Household consumption							
Henriksdal	Large STP, households, industries and storm waters 640 000 pe		X			X	
Vimmerby	Small STP, mixed 43 000 pe		X			X	

9.2 Regional

Regional programmes were designed by the three County Administrative Boards that participated in the study: Jönköping, Värmland and Skåne. As described below, most regional samples cover one or two substance groups.

9.2.1 Jönköping

The strategy was to study municipal STPs with respect to incoming water, sludge, effluents and surface sediments in the corresponding recipients. One large and three smaller STPs were studied (Table 20). In addition, three storm waters were taken in an area influenced by road traffic. This programme covered tertiary butylphenols and methylphenols.

Table 20. Municipal sewage treatment plants studied in the Jönköping county.

STP	Characteristics	pe	Corresponding recipient	Possible additional sources to the recipient
Landsbro	mainly household and storm water	2 100	Gröpplebäcken	
Gislaved	industries (plastics and metal)	20 000	Nissan, Gislaved	
Jönköping	urban storm water, paper industry	85 000	Munksjön	large city, paper industry
Hultsfred	wood industry, storm water	10 000	Hulingen	

9.2.2 Värmland

This is the only regional programme containing spot samples from industries, mainly sediments. In addition, three municipal STPs were studied (Table 21).

Table 21. Sampling programme for Värmland county.

Matrix	Site	Comment	Analysed substances
INDUSTRIES			
Ground-water	Akzo Nobel, Skoghall	Chemical industry for decades	All
Sediment	Akzo Nobel, Skoghallsådran	Chemical industry with production of chlorine and chlorinated pesticides. Oil in the harbour	Methylphenols
Sediment	Akzo Nobel Skoghall, Anholms V Harbour		Methylphenols
Sediment	Stora Enso, Skoghalls Bruk Emission point	Paper and pulp industry	Methylphenols
Sediment	Billerud AB, Gruvöns Bruk, Grums	Paper and pulp industry	Methylphenols
Sediment	Glafs fjorden, fiber bank; Jössefors industrial area	Former pulp industry (from 1969)	All
SEWAGE TREATMENT PLANTS			
Incoming water	Sjöstads STP in Karlstad		All
Sludge	Sjöstads STP in Karlstad		Tertiary butylphenols long-chain alkylphenols
Sludge	Kristinehamn		Tertiary butylphenols long-chain alkylphenols
Sludge	Arvika		All

9.2.3 Skåne

From the county of Skåne, sewage sludge from ten municipal STPs were analysed. Incoming waste waters were studied for five of these STPs. Five stormwaters from different areas and fish from ten lakes were also analysed. In addition one lake water and one coastal sediment were included (Table 22). This programme covered tertiary butylphenols and long-chain alkylphenols.

Table 22. Sampling programme for Skåne county.

Matrice	Site	Details
SEWAGE TREATMENT PLANTS		
sludge	Bromölla	
sludge	Helsingborg Öresund STP	
sludge	Hässleholm	
sludge	Hörby	
sludge	Landskrona , Lundåkraverket	
sludge	Malmö, Sjölundaverket	
sludge	Perstorp	
sludge	Svedala	
sludge	Trelleborg	
sludge	Ystad	
incoming waste water	Bromölla	
incoming waste water	Landskrona, Lundåkraverket	
incoming waste water	Malmö, Sjölundaverket	
incoming waste water	Perstorp	
incoming waste water	Trelleborg	
URBAN STORM WATER		
Storm water	Hälsingborg, Ättekulla	industrial area
Storm water	Hässleholm,	residential area
Storm water	Malmö	road traffic
Storm water	Perstorp	residential area
Storm water	Ystad, Barnängen,	residential area
LAKES		
Fish	Finjasjön (Hässleholm)	perch muscle
Fish	Fjällfotasjön (Svedala)	perch muscle
Fish	Helsingborg R3	flounder
Fish	Ivösjön (Bromölla, Kristianstad)	perch muscle
Fish	Krageholmssjön (Ystad)	perch muscle
Fish	Spillepeng, Helsingborg	perch muscle
Fish	Storarydsdammen (Perstorp, Klippan)	perch muscle
Fish	Store damm/Fåglasjön (Perstorp, Hässleholm)	perch muscle
Fish	Västersjön/Rössjön (Ängelholm)	perch muscle
Fish	Östra Ringsjön (Höör, Hörby)	perch muscle
ADDITIONAL		
Lake water	Malmö (Vombsjön)	Lake water pump station
Sediment	Helsingborg harbour	

10 Methods

10.1 Sampling

10.1.1 Air sampling

Air samples were collected by pumping air through a glass fiber filter (MG160, Munktell) in series with two glass columns each containing the adsorbents XAD-2 (Amberlite) and polyurethane foam (PUF). The airflow was approximately 1 m³/h. Sampling continued for two weeks. After one week the filter and glass columns were changed. Prior to sampling the filter was heated to 400°C, and the adsorbent columns were cleaned by soxhlet extraction with acetone. The filter and columns were wrapped in aluminium foil and stored in a freezer (-18°C) until analysed.

10.1.2 Sludge sampling

The staff at the different treatment plants collected the sludge samples from the anaerobic chambers. The sludge was transferred into pre heated (400°C) glass jars fitted with aluminium foil lined screwcaps and stored in a freezer (-18°C) until analysed. Some samples were stored at 4°C after addition of sodium azide (2 g/l).

10.1.3 Sediment sampling

Surficial sediment (0-2 cm) samples were collected by means of a Kajak sampler. The sediment was transferred into pre heated (400°C) glass jars fitted with aluminium foil lined screwcaps and stored in a freezer (-18°C) until analysed.

10.1.4 Water sampling

The water samples were collected using a Ruttner sampler. The samples were transferred to pre heated (400°C) glass bottles and acidified with H₃PO₄. The samples were stored at 4°C until analysed.

10.1.5 Fish samples

The fish samples from Skåne were collected by means of fishing net, hoop net or fishing-rod. Samples of herring from Fladen was supplied from The Environmental Specimen Bank and the Swedish Museum of Natural History (A. Bignert and colleagues). The fish samples were individually wrapped in aluminium foil and stored in freezer (-20°C) until analysed.

10.2 Analysis

10.2.1 Chemicals

The solvents, HPLC-quality, acetone, hexane, pentane, methyl-*tert*-butylether (MTBE) were delivered from Rathburn (Chemical Ltd., Peeblesshire, Scotland). Acetonitrile, tetrahydrofuran (THF) dichloromethane (DCM) and 2-propanol were delivered from J. T. Baker (Gross-Gerau, Germany). The solvents THF and DCM were not stabilised by any phenolic antioxidants.

Modified diatomaceous earth and solid phase columns (C18, ENV+ and aminopropyl) were delivered from IST (International Sorbent Technology Limited, UK). The phenol 2,6-di-*tert*-butyl-4-methylphenol (BHT) was detected in high amounts in all three SPE-columns. Different trademarks were tested and the conclusion from this investigation was that BHT is a common artefact in SPE-phases and columns. It was therefore necessary to pre-clean the columns prior use by washing them with different solvents. The ENV+ column was especially difficult to clean but acceptable result were obtained by repeated wash with THF.

Sodium sulphate, sodium chloride, silica gel and zinc powder was delivered from Merck. Sodium sulphate, sodium chloride and silica gel were pre heated (400°C) prior use. Acetic acid anhydride, pyridine and 4-diaminopyridine (4-DMAP) were delivered from Fluka (Buchs, Switzerland). All solvents, chemicals and equipment were checked by GC-MS before use. These blanks commonly contained BHT in low to negligible amounts. 3-methyl-6-chlorophenol and 3-ethyl-4-chlorophenol were used as surrogate standards.

Ultra pure water was produced by a Milli-Qplus (Millipore Corporation, Bedford, MA, USA)

10.2.2 Extraction of air samples

The filter and glass columns were Soxhlet extracted with acetone containing ascorbic acid for 24 h. The acetone was concentrated on a Rotavap (Büchi Switzerland), spiked with surrogate standards and diluted with ultra pure water to a final concentration of 25 % acetone in water. The mixture was extracted with pentan : MTBE (1:1) three times. The combined extracts were dried over sodium sulphate, concentrated and cleaned up as described below. The procedure is schematically described in Figure 11.

10.2.3 Extraction of sludge and sediment samples

The samples were thawed and mixed carefully after the addition of ascorbic acid. The water in the sediment and sludge samples was separated by centrifugation before the extraction. Surrogate standards were added to the sediment and sludge. Three consecutive acetone extracts were combined. The acetone was diluted with ultra pure water and extracted twice with a mixture of pentane and MTBE. The extract was subjected for clean up and derivatization (described below) prior GC-MS analysis. The procedure is schematically described in Figure 12.

10.2.4 Extraction of water samples

The water samples spiked with surrogate standards were concentrated by means of SPE-columns (ENV+). Most of the water samples were filtrated (pre heated GF/C-filter) before SPE-concentration due to the high content of particulate material. The filter was extracted separately.

The SPE-column was cleaned and activated prior use with tetrahydrofurane and dichloromethane. The flow rate during extraction was 25 ml/min. The analytes were eluted from the SPE-column with tetrahydrofurane.

Some of the analytes, *e.g.* nonyl-, oktyl- and *tert*-butylphenols, have a tendency to adhere to glass surfaces (Rudel et al., 2003; Wenzel et al., 2004). It was therefore necessary not only to extract the water sample but also to rinse the sample bottle with organic solvent. The extracts were combined.

The combined extract was diluted with water and extracted three times with pentane : MTBE (1:1). This extract was subjected to clean up (described below). The procedure is schematically described in Figure 13.

10.2.5 Clean up of air, sludge, sediment, and water samples

Large amounts of natural organic compounds are co-extracted with the analytes. An easy and effective method to separate a great deal of these non target compounds was to shake the extract with a carbonate buffer (pH 10). At this pH the analytes remained in the organic phase but many acidic and more polar compounds were extracted into the carbonate phase. The carbonate extract was discarded. The cleaned up extracts were derivatized as described below.

10.2.6 Extraction and clean up of fish samples

The fish samples were thawed and subcutaneous muscle tissue were dissected and used for analysis. The samples were spiked with surrogate standards and extracted according to Jensen (1972) and the lipid content was determined according to Jensen (2003).

Clean up of fish extract was performed in two steps. The first step separated the bulk amount of the lipids by means of a column prepared with modified diatomaceous earth on the top of a C18-column using acetonitrile as mobile phase. The eluate (acetonitrile) was diluted with ultra pure water and extracted, dried and concentrated. The remaining lipids, mainly free fatty acids, were removed on an SPE-column containing an amino propylene phase. MTBE containing 10 % 2-propanol was used as mobile phase.

The extract was subject to derivatization and silica gel clean up (described below) prior GC-MS analysis. The procedure is schematically described in Figure 14.

10.2.7 Derivatization

All phenols in this investigation but the shielded 2,6-*tert*-butylphenols are possible to derivatize. We decided to derivatize the non-shielded phenols for two reasons: (a) improved clean up of the extract, (b) improved chromatographic properties and separation on the GC-column.

Three derivatives of the phenols were studied: *O*-methyl ethers, *O*-acetate and *O*-trimethyl silyl ethers. The most suitable derivative was the *O*-acetates since: (a) all non-shielded phenols could be derivatized and (b) the acetylated phenols are stable enough to be chromatographed on a silica column. This results in cleaner extracts and the option to separate the extract in two fractions: shielded not acetylated (2,6-di *tert*-butylphenols) and acetylated phenols.

Most of the phenols are smoothly acetylated using pyridine as base. Some phenols need a stronger base. In this case the 4-DMAP was the base of choice making it possible to acetylate even the quite shielded 6-*tert*-butyl-2,4-dimethylphenol.

The 2,6-*tert*-butylphenols and *tert*-butylhydroquinone are susceptible to oxidation during the derivatization. This could be mastered by adding a small amount of zinc powder (“reductive acetylation”, Vogel 1970) and evacuate the oxygen by flushing the test tube with nitrogen.

10.2.7.1 Acetylation

The extract, in a test tube, was dissolved in hexane: MTBE. Acetone, zinc powder, acetic acid anhydride, and the base (pyridine containing 4-DMAP) was added. The

oxygen was evacuated by flushing the test tube with N₂. The reaction was accomplished on a heating block. The excess reagents were removed by shaking the extract with water. The derivatized extract was dried over sodium sulphate and finally subjected to clean up on a silica gel column.

10.2.8 Silica gel chromatography

A deactivated silica gel column was prepared in a Pasteure pipette. The underivatized phenols (2,6-di-tert-butylphenols) were eluted with hexane. The acetylated phenols were eluted by hexan containing MTBE. Internal standard (octachloronaphthalene) was added to the extracts prior to analysis by GC-MS.

10.2.9 GC-MS analysis

The extracts were analyzed on a 6890N gas chromatograph with a 5973N mass selective detector (Agilent). The injection was done in pulsed splitless mode at 250°C. The fused silica capillary column (VF-5MS 30 m x 0,25 mm i.d. x 0,25 µm film thickness, Varian) was held at 50°C for 3 min., ramped 12°C/min to 300°C and held at 300°C for 10 min. Helium was used as carrier gas. The mass spectrometer transfer line temperature was 280°C. The detector was used in selected ion monitoring mode with electron ionisation at an energy of 70 eV. The analytes were identified by their characteristic retention time and one quantification ion and in most cases one or two supporting ions used to increase specificity was recorded (see Table 23). Quantification was based on comparison of peak abundance to the known response of the internal standard (octachloronaphthalene). The reported analyte concentrations were corrected according to the determined surrogate standard losses.

Table 23. Type of derivative, target and qualifier ions used for GC-MS
analysis of the different analytes. ac = O - acetylated.

	Derivate	Target ion	Qualifier ion(s)
2-tert-Butylphenol	ac	135	107, 150
4-tert-Butylphenol	ac	135	107, 150
2,6-Diisopropylphenol	ac	163	178
6-tert-Butyl-2,4-xylenol	ac	163	178, 135
tert-Butyl-4-hydroxyanisole	ac	165	180
2,4-Di-tert-butylphenol	ac	191	206
Isoeugenol	ac	164	206
tert-Butylhydroquinone	ac	166	151
4-tert-Butyltoluen		133	150, 148
2,6-Di-tert-butylphenol		191	206
2,6-Di-iso-butylphenol	ac	206	177
2,6-Di-tert-butyl-4-methylphenol		205	220
2,6-Di-tert-butyl-4-ethylphenol		219	234
2,4,6-Tri-tert-butylphenol		247	262
2-Methylphenol	ac	108	107, 150
3-Methylphenol	ac	108	107, 150
4-Methylphenol	ac	108	107, 150
2,4-Dimethylphenol	ac	122	107, 164
3,5-Dimethylphenol	ac	122	107, 164
2,3-Dimethylphenol	ac	122	107, 164
3,4-Dimethylphenol	ac	122	107. 164
4-n-OP	ac	206	107
4-tert-OP	ac	135	177
4-tert-OP-EO1	ac	87	221
4-tert-OP-EO2	ac	265	87
4-n-NP	ac	107	220
4-NP (isomeric mixture)	ac	135/149	107/135/149
4-NP-EO1 (isomeric mixture)	ac	87	
4-NP-EO2 (isomeric mixture)	ac	87/265	
4-DP (isomeric mixture)	ac	135	

10.2.10 Quality control

Acetone with ascorbic acid was spiked with the analytes to check the stability during soxhlet extraction. The analytes were quantitatively recovered.

The recovery of the analytes from spiked sediment and sludge samples were determined. The recovery rate of the tert-butylphenols analysed as *O*-acetates was 78-124% with the exception of the easily oxidised tert-butylhydroquinone (58%). The recovery of the non-acetylated tert-butylphenols were in the range 46-82%.

The LODs were determined by a combination of deviation of blanks and judgement of noise levels in the actual sample chromatograms.

The most frequently detected artifacts in the blank samples were nonyl phenols and 2,6-di-tert-4-methyl-phenol which is in agreement with what has previously been reported (Oros and David, 2002; Rudel et al., 2003, Wenzel et al., 2004). The most important source of 2,6-di-tert-butyl-4-methylphenol was equipment made of plastic. Therefore, equipment made of plastic was avoided as far as possible and substituted for the equivalent made of glass. All glass equipment, glass fiber filters, sodium sulphate and sodium chloride was cleaned by heating to 400°C for 4 h prior to use. All other equipment was washed with organic solvent before use. In spite of these precautionary measures, the data on 2,6-di-tert-butyl-4-methylphenol, especially at low concentrations close to LOD, should be used with caution.

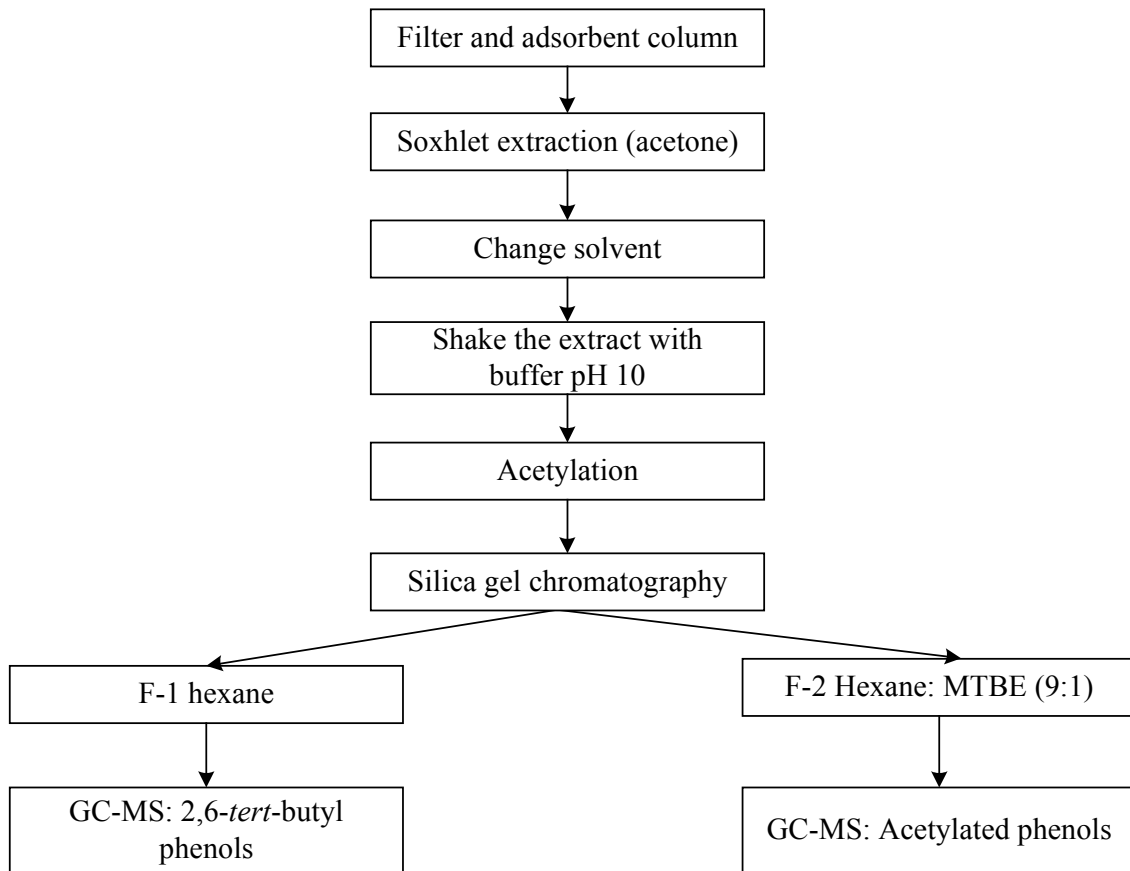


Figure 11. Analytical scheme: air samples

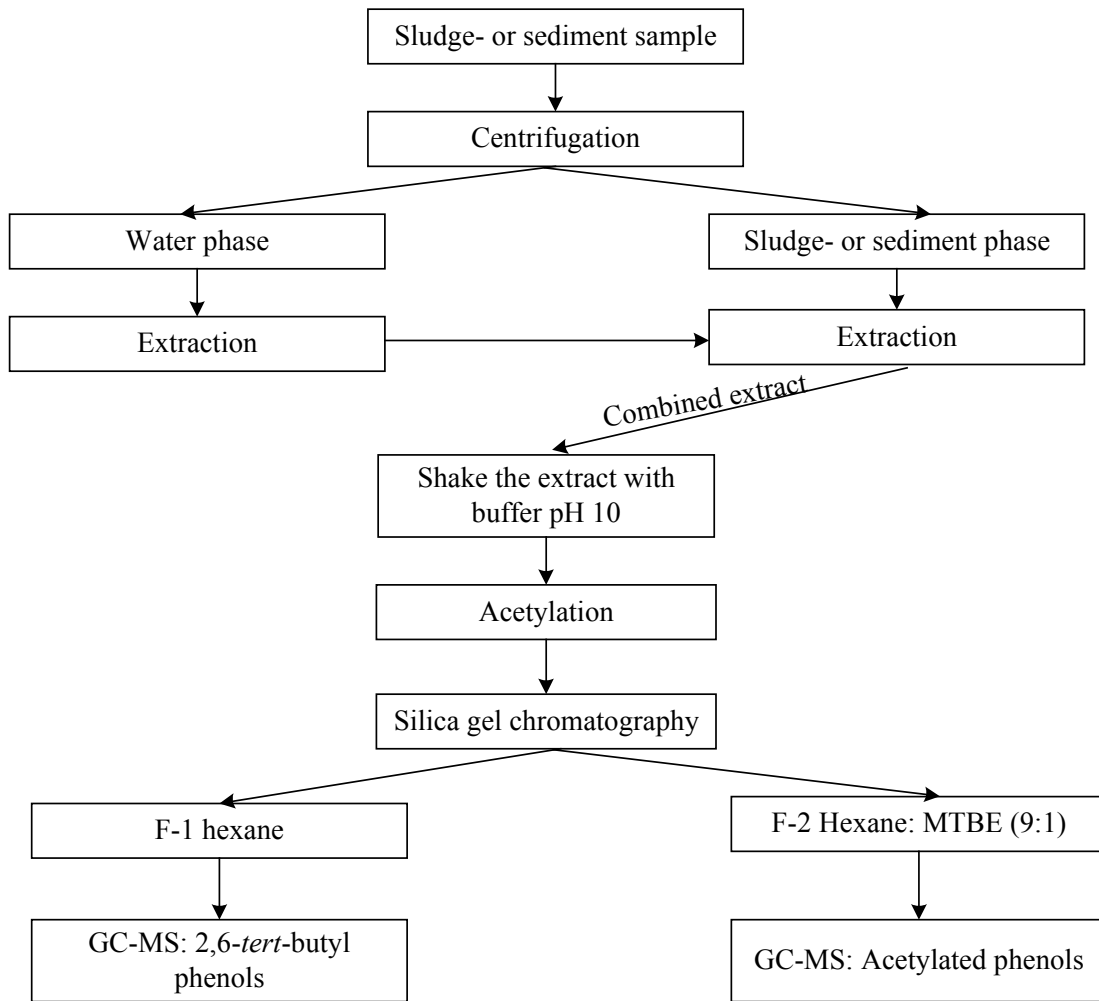


Figure 12. Analytical scheme: sludge- & sediment samples.

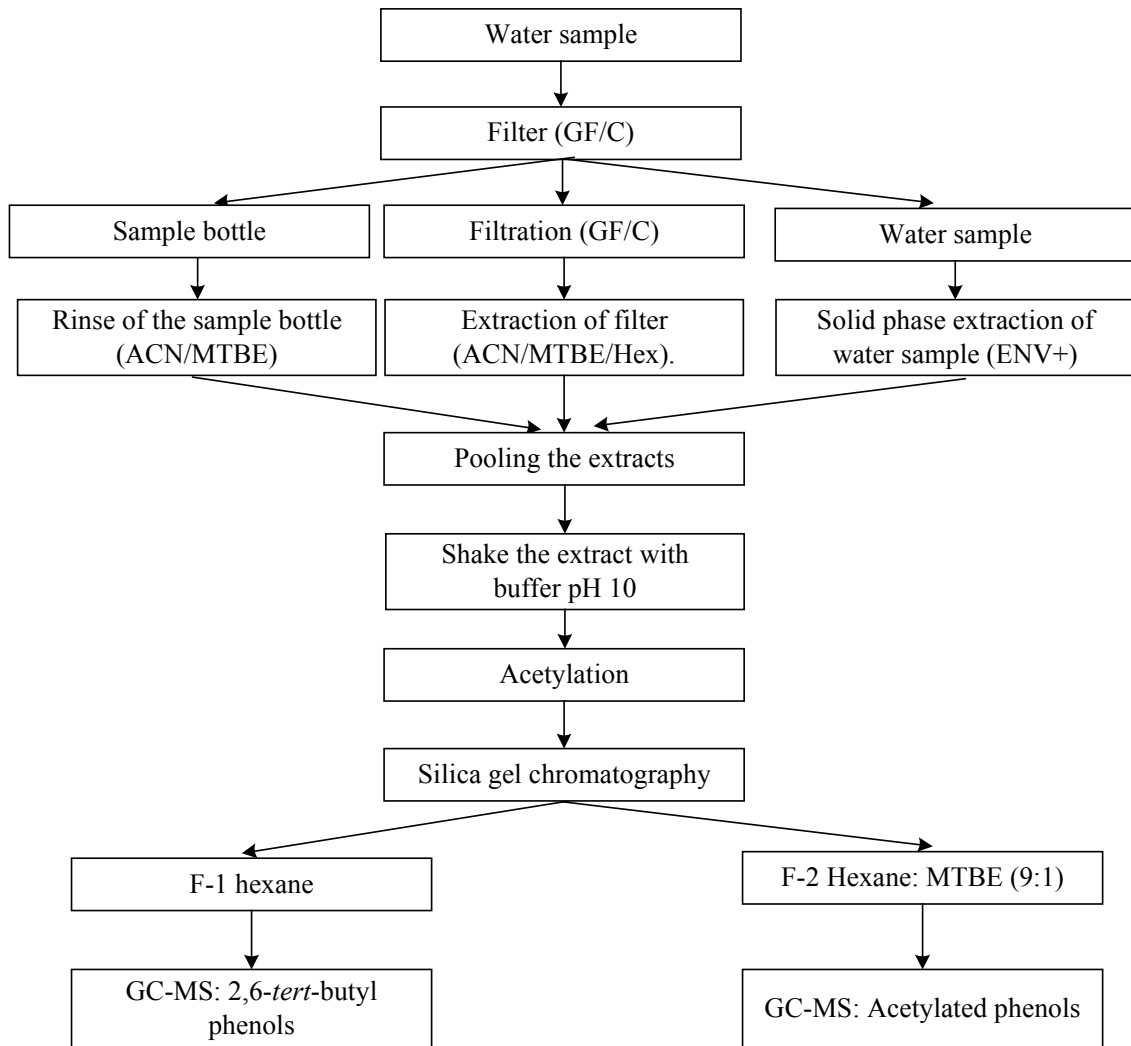


Figure 13 Analytical scheme: water samples

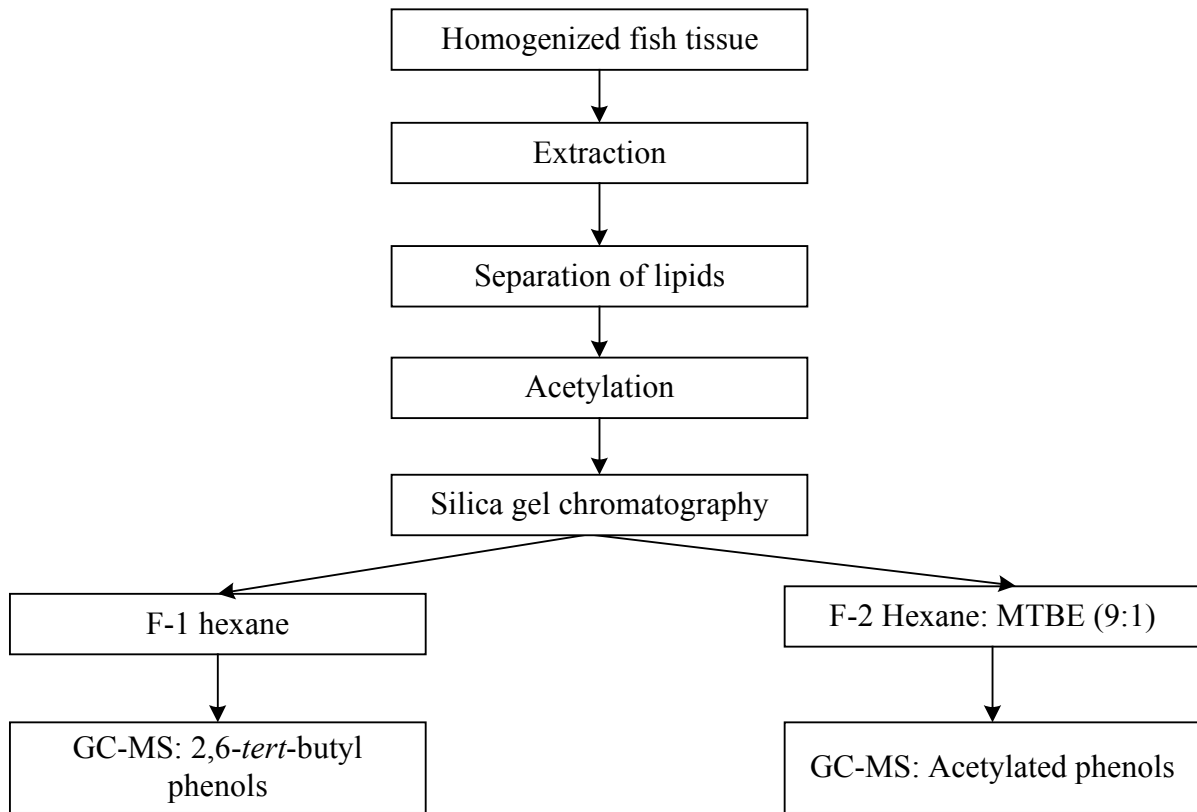


Figure 14. Analytical scheme: fish samples

11 Results

This chapter presents an overview of data with detection frequencies and concentration ranges. All results are listed in appendix (Table A 7 through Table A 18). A screening typically results in very few samples per site and matrix, poorly reflecting the variability of concentrations. We will first illustrate the variability of levels, using some samples that were taken in triplicate. At two sites (upstream and downstream a chemical industry), surface sediments were taken in triplicate within a radius of ca 50 m. Sludge from four municipal STPs were also sampled in triplicate. Relative standard deviations are summarised in Table 24. All data and relative standard deviations for the sediments are shown in Table A 20, in the appendix. Most upstream data are < d.l.. For the long-chain alkylphenols, the variability is much higher in sediments than in sludge. This is also true but less pronounced for the other substances. This reflects the heterogeneous nature of sediments. However, because the variability differs widely between the substances, analytical and sampling uncertainty is also likely to contribute to the observed variability between triplicate samples.

Table 24. Variability of triplicate samples, as median values of the relative standard deviations. Ranges of individual values in brackets. Many substances were <d.l., in particular in the sludge samples. When less than four compounds in each group were > d.l., no average values were calculated.

Matrice	Site	Rel. Std dev. Tert butylphenols	Rel. Std dev. Metylphenols	Rel. Std dev. Long-chain alkylphenols
Sediment	Downstream chemical industry	median 34% (3.5-84 %)	Median 38 % (20-55 %)	median 63 % (21-88%)
Sludge	Henriksdal, composite daily samples from 3 following days	(10-21 %)	8%, 52 %	median 17% (5-22 %)
Sludge	Stenungsund, three composite samples from one day	median 18 % (6-82 %)	Median 30% (5-65 %)	median 10 % (3-13%)
Sludge	Vimmerby, composite daily samples from 3 following days	Median 16 % (12- 39%)		median 9 % (8-43%)
Sludge	Vimmerby, composite daily samples from 3 following days	Median 8 % (5-14 %)	Median 45 % (10-92 %)	median 9 % (2-13 %)

The concentration ranges and the detection frequencies of individual compounds are presented in Figure 15 - Figure 20. Concentrations in background, industrial, STP recipient and urban sediments are also presented separated in the different categories (Figure 17 and Figure 18).

Detection limits vary between samples and are occasionally higher than many detectable levels due to individual matrix effects (Table A 20). The concentration ranges presented in Figure 15 - Figure 20 do thus not include samples below d.l. Consequently, the concentration ranges do not represent the entire investigated population. For substances with low detection frequencies, the concentration range is probably biased.

Additionally, ten fish samples were analysed for tertiary butylphenols and long-chain alkylphenols, whereas three samples of herring from Fladen were analysed for all compounds. The branched 4-NP was detected in perch from one lake at 15 ng/g ww, slightly above the d.l. and 4-t-OP in perch in another lake at 1.3 ng/g ww. None of the other substances were detected in any fish sample.

Three soil samples were taken in an industrial area (Trollhättan). Six out of seven methylphenols were detected at levels of a few ng/g dw, except for 4-methylphenol that occurred at ca 20 ng/g dw. Of the tertiary butylphenols, only 4-t-butylphenol and 2,4-di-t-butylphenol were above d.l., and occurred at ca 1 ng/g dw. Of the long-chain alkylphenols, 4-t-octylphenol and 4-nonylphenol were detected at ca 1-2 and 11-60 ng/g dw, respectively.

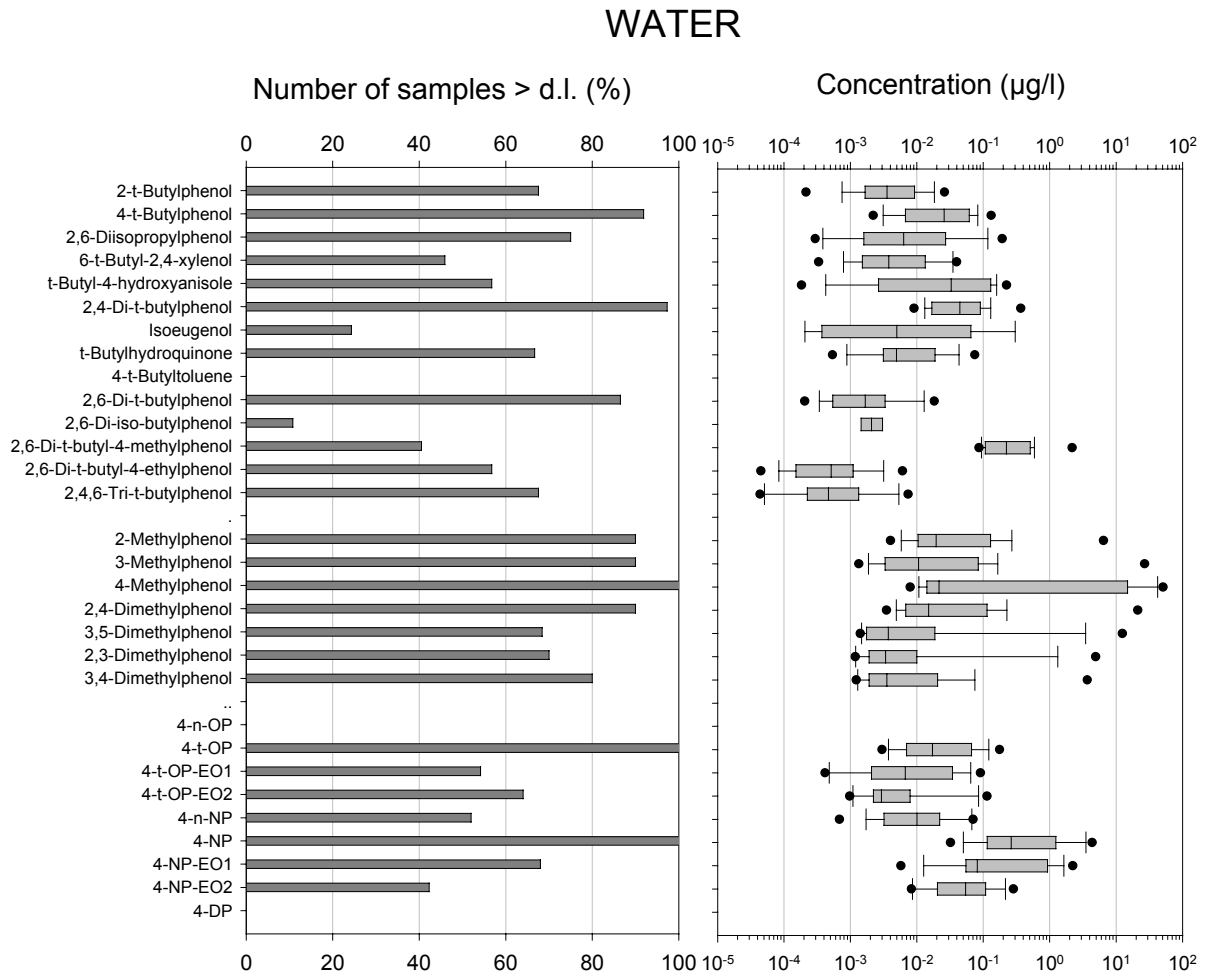


Figure 15. Water samples: detection frequencies and concentration distributions. The samples include surface waters, STP influents and effluents and storm waters. Note that all compounds were not analysed in all samples, why the detection frequency is given as % rather than in absolute numbers.

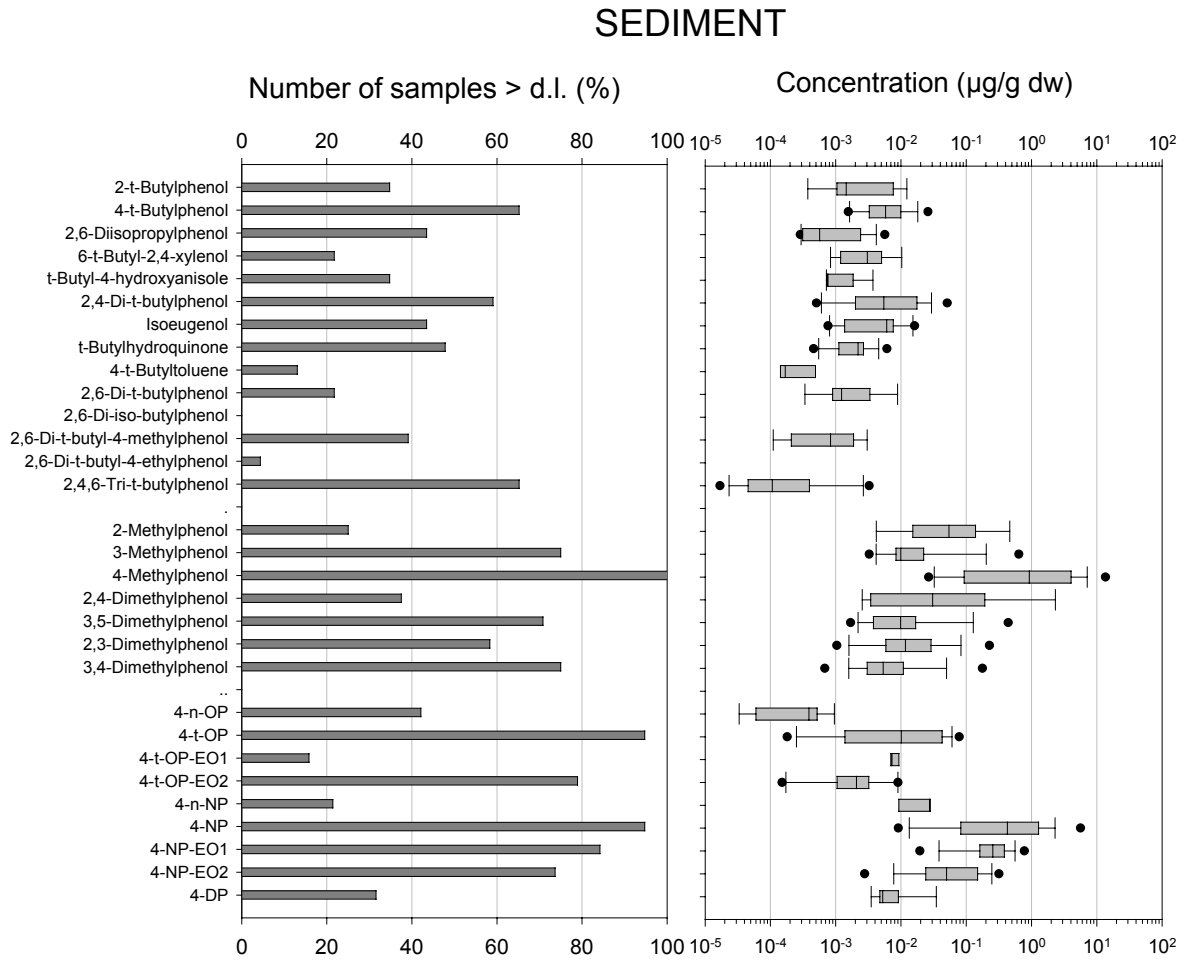


Figure 16. Sediment samples: detection frequencies and concentration distributions. Note that all compounds were not analysed in all samples, why the detection frequency is given as % rather than in absolute numbers.

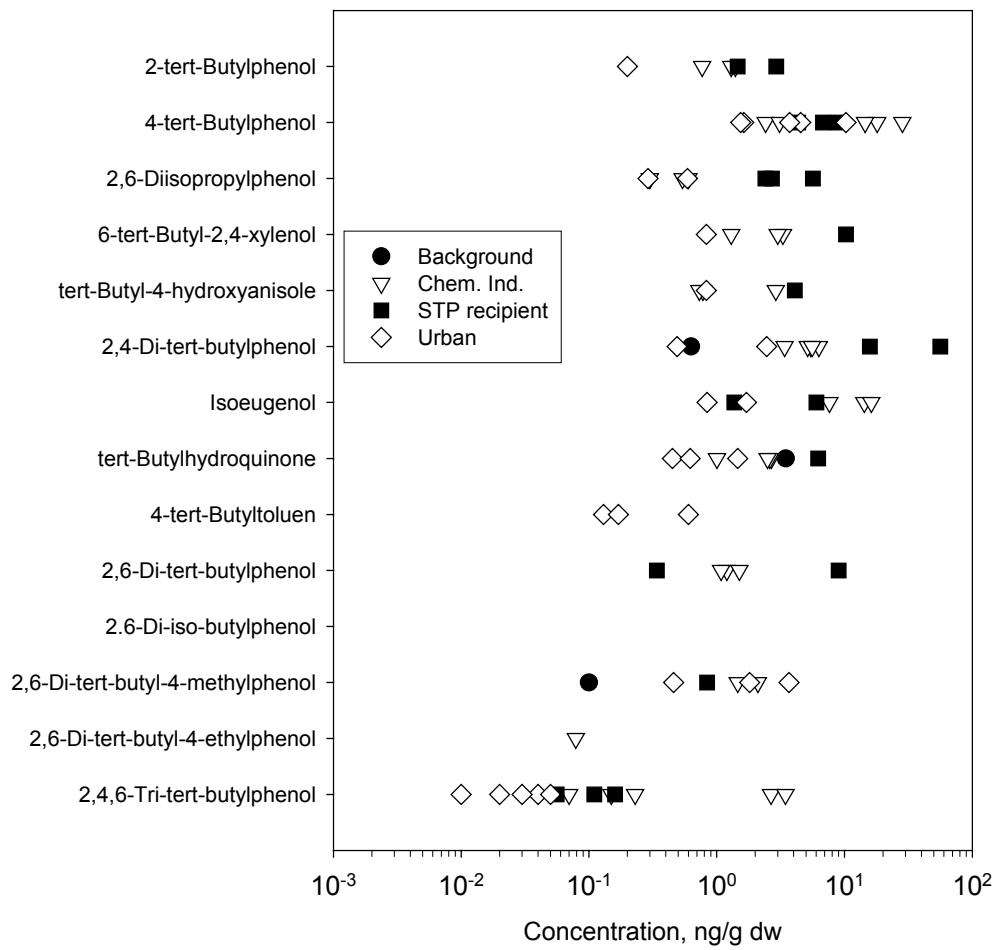


Figure 17. Tertiary butylphenols and related compounds in sediments from different type regions. Four sampling sites have been excluded in the graph. Please note that levels are expressed in ng/g dw.

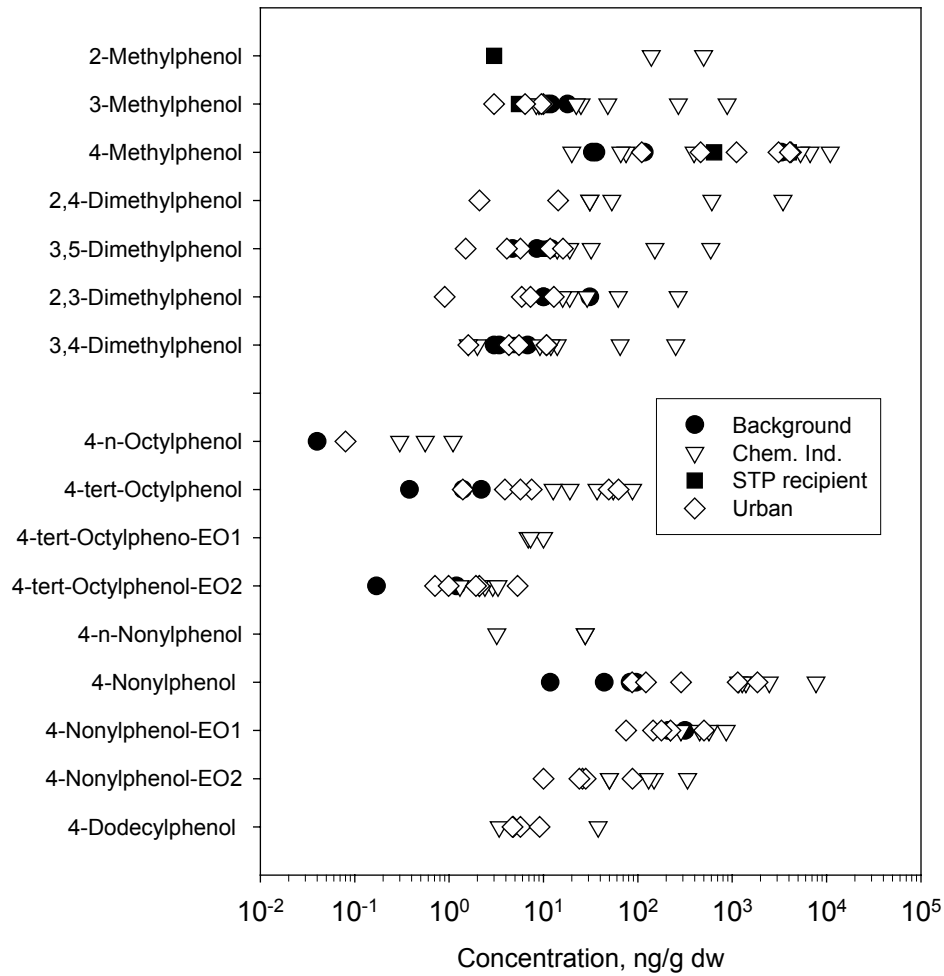


Figure 18. Methylphenols and long-chain alkylphenols in sediments from different type regions. Please note that levels are expressed in ng/g dw.

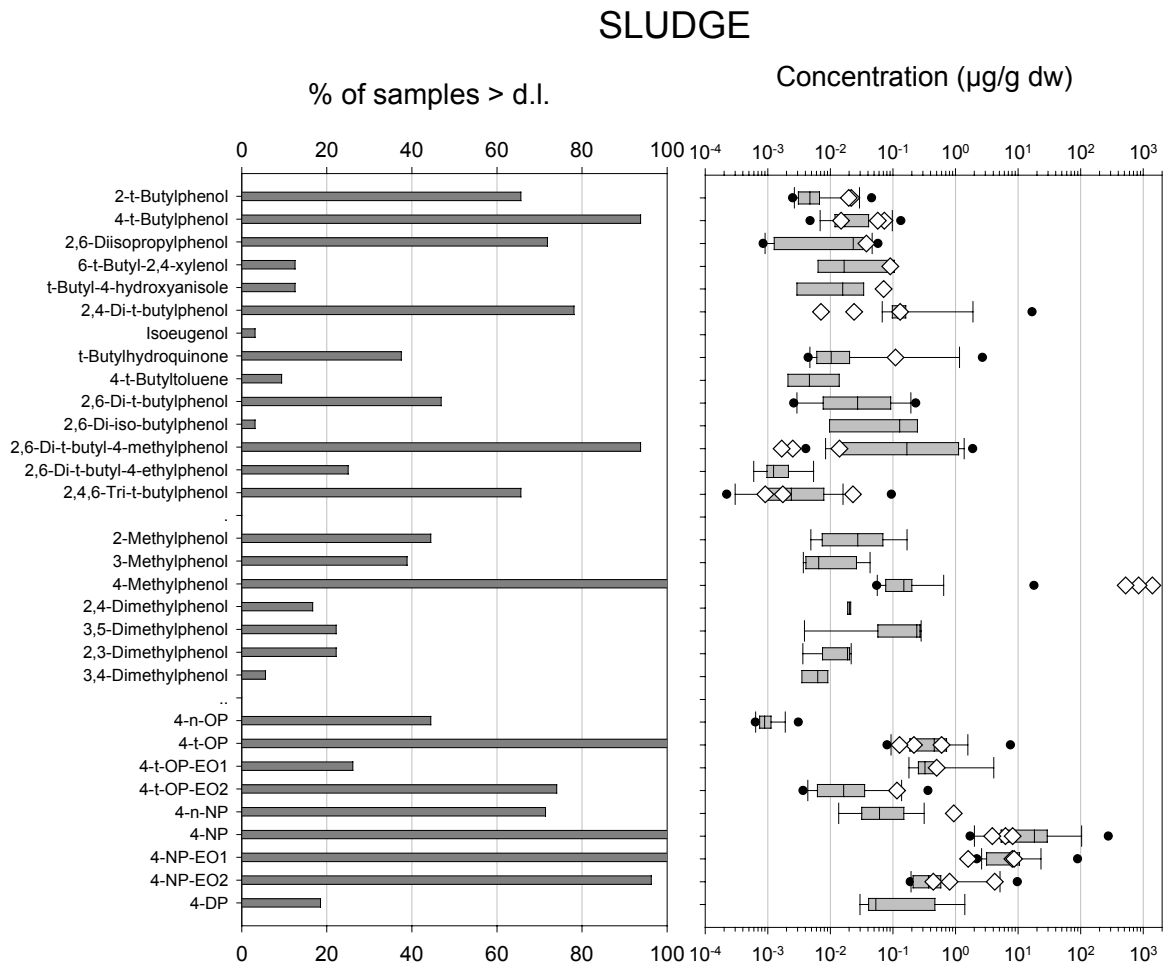


Figure 19. Sludge samples: detection frequencies and concentration distributions. The box-whisker plots represent the 29 municipal STPs, and the diamonds represent three samples from an industrial STP. Detection frequencies are in % because all compounds were not analysed in all samples.

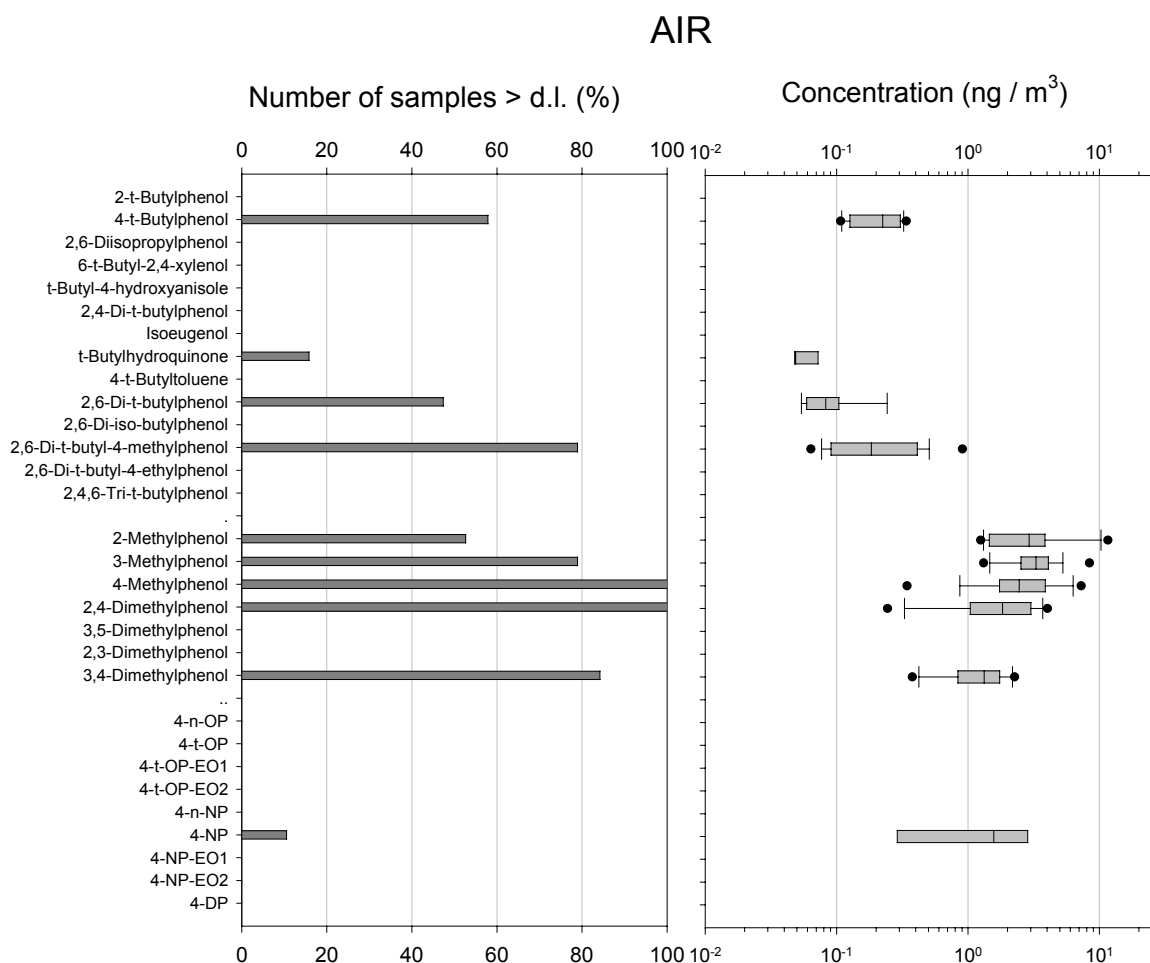


Figure 20. Air samples: detection frequencies and concentration distributions. Detection frequencies are in % because all compounds were not analysed in all samples.

11.1 Tertiary butylphenols

Most tertiary butylphenols and the related compounds were detected in sediments, water and sludge, but never in fish. Detection frequencies vary widely in sludge and sediments. In air, only the four most commonly used substances were detected: 4-t-butylphenol, 2,6-di-t-butylphenol, 2,6-di-t-butyl-4-methylphenol and occasionally t-butylhydroquinone¹. Levels in municipal sludge commonly vary by more than two orders of magnitude, and occasionally exceed 1 µg/g dw. The levels in sediments also span over one to two orders of magnitude for individual substances.

¹ In the environment, tert-butylhydroquinone may undergo reversible oxidation (see chapter 8.1). Thus, this chemical is reported as the sum of the oxidised and the reduced forms.

11.2 Methylphenols

The methylphenols were abundant both in terms of detection frequencies and concentrations. The monomethylated phenols generally occur at higher levels than the dimethylated phenols. Levels in air generally exceeded 1 ng/m³. 2-, 3- and 4-methylphenol occurred at similar levels in air, whereas other media commonly showed 4-methylphenol > 2-methylphenol > 3-methylphenol. This contrasts with the registered use, where 3-methylphenol is by far the major substance (chapter 5). 4-methylphenol in sediments often exceeds 1 µg/g dw. It was not possible to evaluate the chromatograms for two of the dimethylphenols in air. In contrast to tert butylphenols and long-chain alkylphenols, methylphenols generally occur in lower concentrations in the sludge samples than in the sediments.

11.3 Long-chain alkylphenols

Octyl- and nonylphenols and their ethoxylates were detected in most samples of water, sediment and sludge. Dodecylphenol was less abundant than 4-t-OP or 4-NP in sediments and sludge, and was not detected in any water sample, possibly due to the low solubility in water. In air, only 4-NP was detected and then only in two samples.

The major compounds detected are 4-t-OP and 4-NP, which were detected in almost every sample of water, sludge and sediment. Their corresponding ethoxylates were also commonly detected. The straight chain isomers 4-n-OP and 4-n-NP were detected fairly frequently, but at much lower levels than the major isomers. We are not aware of any studies where the straight chain isomers have been detected in environmental samples. According to ECB (2002), 4-n-NP is not used in Europe. Although the Products Register (or SPIN) contains some data on the use of 4-n-NP, it is possible that this actually is the branched 4-NP registered under wrong CAS-number. Hypothetically, the normal alkylchain isomers could be degradation products of other substances.

12 Discussion

12.1 Background regions

Råö and Pallas, where air samples were taken, and Fladen, where fish was collected, are considered as background regions. Furthermore, sediments and lake water from upstream a chemical industry (Perstorp) and a paint industry (anonymous) can be considered to be local background samples, although they are not from remote stations.

12.1.1 Air

The following tert-butylphenols were detected in air from Råö: 4-t-butylphenol, 2,6-di-t-4-methylphenol and, in one sample close to d.l., 2,6-di-t-butylphenol. 2,6-di-t-4-methylphenol was also found in Pallas. These are the high volume chemicals in this group. The 4-methylphenol and two of the dimethylphenols were also detected in Råö, and some of these substances also in Pallas but at lower levels. Methylphenols have an estimated atmospheric half-life of ca 5 hours (Table A 19). Their presence in Pallas is therefore a little unexpected and may indicate that they are formed in the region, e.g. by direct emissions from wood stoves or through oxidation of toluene. None of the long-chain alkylphenols were detected in background air.

12.1.2 Fish

None of the substances were detected in herring from Fladen on the Swedish west coast.

12.1.3 Sediments

Four sediments taken upstream two industries in southern Sweden serve as local background. Only three positive identifications of tertiary butylphenols were made, close to 1 ng/g dw. Most methylphenols were detectable in the range 3-35 ng/g dw, except one sample that was high in 4-methylphenol (3300 ng/g dw). Of the long-chain alkylphenols, 4-NP and 4-NPEO1 were fairly abundant (10-300 ng/g dw) whereas 4-t-OP occurred at ca 1 ng/g dw.

12.2 Municipal sewage treatment plants

Samples from municipal STPs cover 29 samples of sludge, 10 samples of incoming waters and 10 effluents. A further three sludge samples came from the STP of a major

chemical industry, and six effluents were taken at two industrial STPs. These industrial samples are discussed in chapter 12.3.

The total concentration ranges in sludge are shown in Figure 19. In terms of both level and detection frequency, the most abundant compound is 4-NP and its precursors. 4-NP is a major pollutant in Swedish STPs and is regularly measured. Other abundant pollutants in this study are 4-t-OP, 2,6-di-tert-butyl-4-methylphenol, 2,4-di-tert-butylphenol, 2,6-di-tert-butylphenol and 4-methylphenol. Certain substances show fairly high levels but low detection frequencies, e.g., 3,5-dimethylphenol and 2,6-di-isobutylphenol. 2,4-di-t-butylphenol display one extremely high value in sludge (Ystad).

The levels in sewage influents and effluents in the municipal STPs are illustrated in Figure 21. By far the most common substance in the influents is 4-methylphenol, followed by 4-NP, 4-NP-EO1, 2,3-dimethylphenol, 3,5-dimethylphenol and 2,6-di-t-butyl-4-methylphenol. Much higher levels of 2,6-di-t-butyl-4-methylphenol (14-42 µg/l) and 4-NP (0.6-37µg/L) were previously detected in Swedish sewage influents (Paxeus, 1999). High levels of 2,6-di-t-butylphenol (25-145 µg/L) were also detected in the study by Paxeus, (1999), which is many times higher than in the current study, where it was generally lower than 0.02 µg/L.

Although most of the influent/effluent data are not from the same STPs, Figure 21 indicates that most substances are efficiently retained or degraded in STPs. Effluent/influent ratios can be calculated for four individual STPs covering data on tert butylphenols and methylphenols. Results for some of the substances occurring at highest levels show that the apparent effluent/influent ratios vary widely for each substance (Table 25). 4-methylphenol occurs at very high concentrations in some sewage influents (Jönköping and Landsbro), but is apparently efficiently degraded in these STPs, which is in agreement with experimental results (e.g., Boyd et al., 1983).

Table 25. Effluent/influent ratios (%) for selected substances in four STPs.

STP	Unit	4-t-butyl-phenol	2,6-diiso-propylphenol	2,4-di-t-butylphenol	2,6-di-t-butyl-4-methylphenol	4-methylphenol
Gislaved	%	120%	29.0%	67.4%	3.5%	no data
Hultsfred	%	31%	3.8%	23.6%		no data
Jönköping	%	19%	0.3%	0.3%	82%	0.1%
Landsbro	%	32%	28%	14%		0.1%

Water from non-industrial STPs

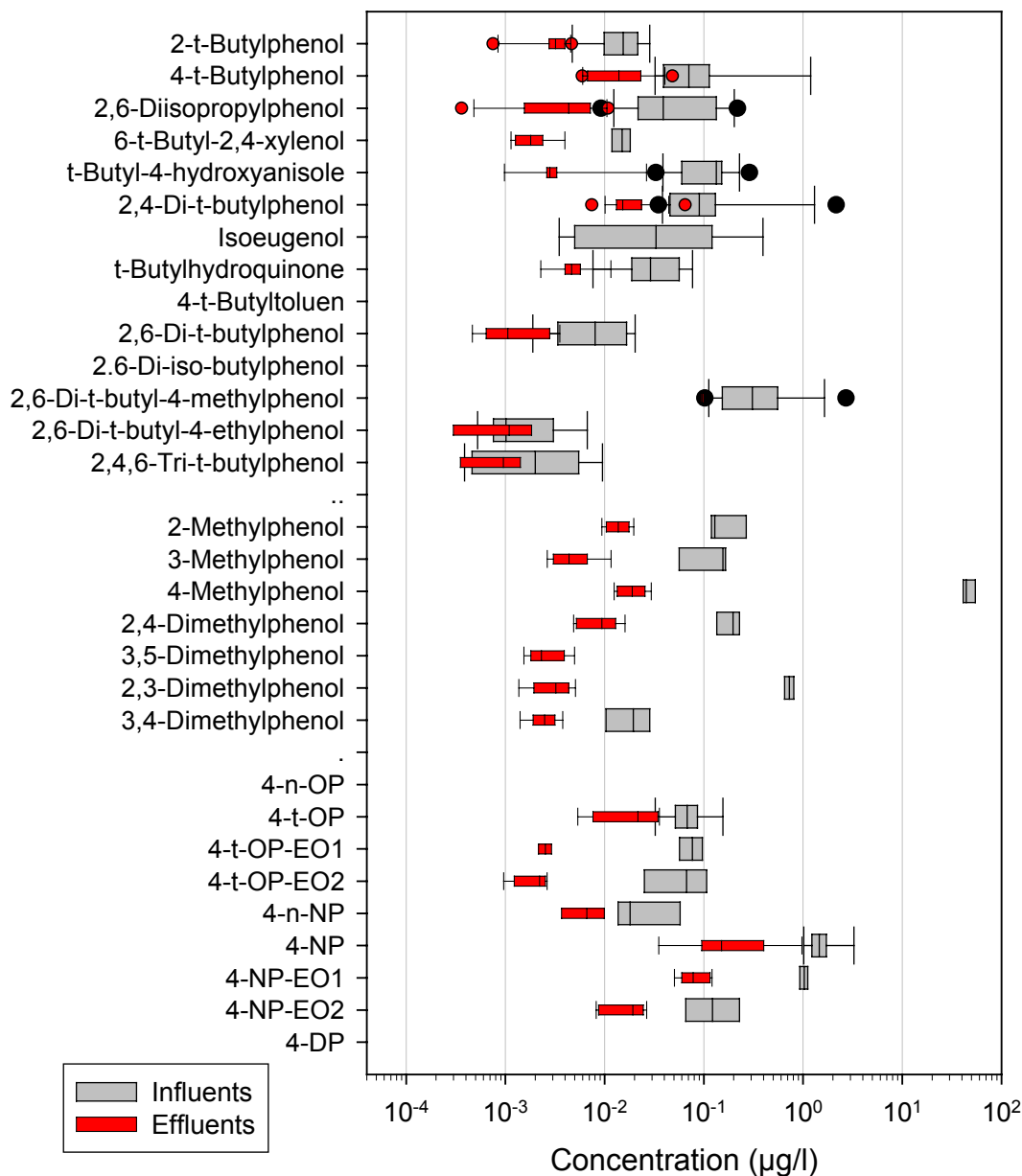


Figure 21. Concentrations in inflows and effluents of municipal sewage treatment plants.

In order to assess the possible impact of storm water runoff to the total load of STPs, the ratios between the median concentration in storm water and the median concentration in sewage influent were calculated for all chemicals. It should be emphasised that the few samples of storm water available do not reflect the dynamics of storm water, thus the assessment should be treated with caution, and merely as indication of possible impact. Methylphenols were not analysed in storm waters. The concentrations of tertiary butyl-

phenols and long-chain alkylphenols in storm waters are typically about one order of magnitude lower than in sewage influents. The ratios of the median levels lie in the range 0-0.6 (median 0.05), with 2,4-di-t-butylphenol displaying the highest ratio. This limited assessment does not suggest that storm water has a major impact on the total STP loads of these chemicals.

12.2.1 Tertiary butylphenols

Many of the tertiary butylphenols are used as antioxidants in various common products and can be expected to occur in sewage sludge due to input from households. Abundance in sludge from municipal STPs agrees fairly well with data on the amounts used (chapter 4). The “high-volume” chemicals 2,6-di-t-butyl-4-methylphenol, 2,6-di-t-butylphenol and 4-t-butylphenol all show high detection frequencies and are relatively abundant in the sludge samples. Several compounds for which there is no or very low reported use in the Products Register (t-butyl-4-hydroxyanisole, 4-t-butyltoluene, isoeugenol, 2,6-di-t-butyl-4-ethylphenol and 2,4,6-tri-t-butylphenol) are less frequently detected and occur at lower levels. The agreement between occurrence in sludge and the amount used is not perfect, however. This may be due to e.g. unregistered use, use pattern (household vs industry) and different stability toward degradation in the STPs.

Some of the tertiary butylphenols do intercorrelate pairwise in sludge samples. The statistically significant intercorrelations ($p < 0.05$) are shown in Table 26. In principle, compounds that intercorrelate are the ones that are used in chemical products in Sweden (compare Table 2). The correlation indicates that the relative abundance of those substances in the incoming waters is similar at different STPs. Because industrial load and influence from storm water vary widely between the STPs, the correlation suggests that households rather than industries are major sources.

Table 26. Statistically significant ($p < 0.05$) Spearman correlation coefficients of tert butylphenols and similar substances in sludge from municipal STPs. BP = butylphenols.

	4-t-BP	2,4-Di-t-BP	t-Butyl-hydroQ	2,6-Di-t-BP	2,6-Di-t-butyl-4-MP	2,4,6-tri-t-BP
2-t-butylphenol	0.82	0.59		0.615		0.71
4-t-butylphenol		0.53	0.61			0.71
2,6-Di-isopropylphenol		0.70	0.81	0.71	0.70	0.57
2,4-Di-t-butylphenol				0.65		0.77
2,6-Di-t-butylphenol						0.76
2,6-Di-t-butyl-4-methylphenol						0.70

12.2.2 Methylphenols

Only three samples were analysed for methylphenols in sewage influents, but in all these samples, the levels of 4-methylphenol were very high (40-57 µg/l), both in absolute terms and in relation to the other methylphenols. The enrichment of this specific isomer suggests that it be derived from a common precursor molecule. Intestinal degradation of the amino acid tyrosine partly leads to the formation of 4-methylphenol, which is excreted by urine (Geypens et al., 1997). Levels of total 4-methylphenol (hydrolysed) of 21 ± 21 mg/l have been measured in normal healthy individuals (Nakashima et al., 1998). On the average, this is ca 400 times higher than the levels measured in STP influents. Assuming that a person uses 300 liters of water/day and that the daily urinary production is 1.5 liters, this gives a urine dilution in waste waters that is close to the ratio of 4-methylphenol in urine and in waste waters. Conclusively, the high levels of 4-methylphenol in STP influents may very well be of natural origin.

Levels of the dimethylphenols are generally low, except for 3,5-dimethylphenol that is anomalously high in the three samples from Henriksdal. This STP is influenced by many industries that may possibly explain the presence of this substance.

12.2.3 Long-chain alkylphenols

4-NP is a well known pollutant in sludge from municipal STPs. Levels decreased strongly during the early 1990s and the national average in 2002 was 17 µg/g dw (SCB, 2004). The present data are strongly heterogeneous (Figure 19) and show two clear outliers: Kristinehamn (440 µg/g dw) and Helsingborg (200 µg/g dw), and two less clear outliers (Perstorp, 92 µg/g dw and Ystad, 57 µg/g). The load of 4-NP to these STPs is most likely influenced by industries. Excluding these samples gives an average concentration of 15 µg/g dw. When excluding the outliers, 4-t-OP correlates strongly to 4-NP ($p < 0.0001$; slope 0.025 ± 0.002). This close relation in 12 municipal STPs suggests a diffuse load, and that these compounds are used in and released from similar applications. Other strong correlations between long-chain alkylphenols are shown in Table 27. As could be expected, the alkylphenols and their ethoxylated precursors show some correlation. In sewage influents, no correlation could be established for any of these substances.

The smaller STPs with little or no influencing industry and almost only household waste water seem consistently to display low levels of long-chained alkylphenols in the sewage sludge. Thus, higher levels of alkylphenols in sewage sludge are probably related to storm water and influencing industries.

The presence of 4-n-NP in sludge is puzzling since there is no reported use. There is no correlation between 4-n-NP and 4-NP or the sum of 4-NP + the ethoxylates, neither in sludge, nor in sediment downstream the STPs, suggesting that it is not an impurity of technical nonylphenol (see also chapter 11.3). Dodecylphenol was detected in five STPs, generally close to detection levels. A fairly high level of 1.4 µg/g was detected in the STP of Kristinehamn, which also displayed anomalously high levels of 4-t-OP and 4-NP.

Table 27. Statistically significant ($p < 0.05$) Spearman correlation coefficients of long-chain alkylphenols and similar substances in sludge from municipal STPs.

	4-t-OP-EO2	4-NP	4-NP-EO1	4-NP-EO2
4-n-OP	0.85			0.67
4-t-OP		0.84	0.49	
4-t-OP-EO1	1		0.750	0.83
4-t-OP-EO2				0.7
4-NP			0.60	

12.3 Point sources

As mentioned previously, very few samples are normally analysed per site and matrix in a screening. Lack of knowledge on the local variability of levels will thus limit the possibility of identifying point sources. At one chemical industry, triplicate sediment samples were taken upstream and downstream, within a radius of 50 m at each site, whereby some statistical assessment can be made.

In order to determine whether downstream data were significantly ($\alpha = 0.05$) higher, a t-test or the corresponding non-parametric test was performed for chemicals that were generally $> d.l.$ With this method an industrial impact could be identified only for one substance (3,4-dimethylphenol), although its concentrations differ by only a factor of 2.7 on the average. Unexpectedly, industrial impact of 4-nonylphenol could not be verified statistically although concentrations differ by ca two orders of magnitude. This is due to large variability between triplicate samples, and the low number of samples (3). This analysis illustrates that within a screening, it may be difficult to use statistical methods for verifying concentration gradients. A subjective assessment must be regarded as equally important. Consequently, the following assessment was performed in this manner.

To illustrate the possible environmental impact of potential industrial point sources, samples were taken in the vicinity of industrial sites in the following source categories:

- ✓ Paint industry (anonymous)
- ✓ Chemical industries (Perstorp and Akzo Nobel)
- ✓ Two industrial areas (Trollhättan and Stenungsund)
- ✓ Paper and pulp industry (Stora Enso in Skoghall and Billerud at Gruvön)
- ✓ Four municipal STPs

Most samples were taken in the potentially impacted area, but in Perstorp and at the paint industry, samples were also taken upstream the industry. Table 28 shows a summary of which chemicals that were found in elevated levels on the industrial sites, or in the sediment samples downstream of the industries. It should be emphasised, that this summary is based on very few samples from each industry, and should be treated with caution. A positive mark should be interpreted as an *indication* of industrial impact and not as evidence.

Generally, elevated levels of 4-methylphenol and octyl- and nonylphenols and their ethoxylates were found in the sediments at most sites. The concentrations of 4-methylphenol were, however, high also in upstream samples and natural origin cannot be ruled out. At Akzo Nobel in Värmland, high levels were found of all methylphenols in sediments and groundwater. In groundwater, 4-methylphenol was in the same order of magnitude as in influents to municipal STPs. Chemicals that were elevated in sewage effluents were generally also elevated in sediments, with the exception of 2,6-di-t-butyl-4-methylphenol at the paint industry, which displayed high levels only in sewage effluent. In the industrial area in Trollhättan, the levels of methylphenols were slightly higher than in other cities included in this study. The concentrations were, however, of similar orders of magnitude as measured levels in previous studies (see Table 13). The soil samples from Trollhättan showed a different pattern than the air samples, with slightly elevated concentrations only of 4-methylphenol and 4-NP.

Table 28. As *indication* of *possible* industrial impact, chemicals are shown that were found in elevated levels in samples taken downstream or on industrial sites. An X-mark indicates that a chemical was detected at high levels in one or more matrices, relative to samples in the same matrix from other sampling sites within the study. It should be noted that few samples were taken at each site.

Site	4-t-BP	6-t-butyl-2,4-xylenol	2,4-di-t-BP	2,6-di-t-butyl-4-MP	2,4,6-tri-t-BP	4-MP	Other MP	4-t-OP + EO	4-NP + EO
Paint industry	X	X	X	X	X	X		X	X
Perstorp	X						X	X	X
Akzo Nobel						X	X		
Trollhättan							X		X
Stenungsund									
Billerud						X			
Glafs fjorden						X			X
Stora Enso						X			

Municipal STPs can be regarded as potential point sources. Effluent data do however show fairly low concentrations for most substances (Figure 21). Sediments were taken downstream the four municipal STPs presented in Table 25 and analysed for tert butylphenols and methylphenols. Most substances are below d.l (Table 29). It is difficult to state whether levels are affected by the STPs, since upstream sediment data are lacking. Several of the tert butylphenols are nevertheless higher in these sediments than in central Stockholm.

Table 29. Sediment data (ng/g dw) from downstream four municipal STPs in Jönköping.

	Nissan, Gislaved	Munksjön	Hulingen	Gröpplebacken
<i>corresponding STP</i>	<i>Gislaved</i>	<i>Jönköping</i>	<i>Hultsfred</i>	<i>Landsbro</i>
2-tert-Butylphenol	<0.13	<1.6	2.9	1.5
4-tert-Butylphenol	<0.12	6.8	8.9	4.3
2,6-Diisopropylphenol	<0.11	2.4	5.7	2.7
6-tert-Butyl-2,4-xyleneol	<0.41	<6.9	10.3	<1.8
tert-Butyl-4-hydroxyanisole	<0.19	<2.5	<6.1	4.1
2,4-Di-tert-butylphenol	<0.51	16	56	0
Isoeugenol	<0.26	6	<12	1.4
tert-Butylhydroquinone	<0.32	6.2	<0.6	<1.9
4-tert-Butyltoluen	<0.19	<1	<1.3	<0.68
2,6-Di-tert-butylphenol	<0.13	<0.7	8.9	0.3
2,6-Di-iso-butylphenol	<2	<16	<16	<8.9
2,6-Di-tert-butyl-4-methylphenol	0.8	<8.6	<9.2	<47
2,6-Di-tert-butyl-4-ethylphenol	<0.13	<0.67	<0.83	<0.45
2,4,6-Tri-tert-butylphenol	0.1	0.1	<0.15	0.2
2-Methylphenol		<5.5		3
3-Methylphenol		<2.2		5.5
4-Methylphenol		640		4000
2,4-Dimethylphenol		<23		<9.7
3,5-Dimethylphenol		9.9		<2
2,3-Dimethylphenol		<22		<4.7
3,4-Dimethylphenol		<5.9		5.2

12.4 Urban environment

12.4.1 Sediments

The samples representing urban areas are presented in Appendix (Table A 1). Sediments were studied at two depths, surface and 33-35 cm. The site Essingen is located slightly upstream of central Stockholm, and the other two sites are in central Stockholm. 4-t-butylphenol and 2,4,6-tri-t-butylphenol were detectable in most sediments, whereas most other tertiary butylphenols were detectable in less than three samples. The detection frequencies are higher for most methylphenols and long-chain alkylphenols.

Most tertiary butylphenols occur at less than ca 1 ng/g dw; the highest detected level is 4-t-butylphenol at 10 ng/g. 4-methylphenol occurs at very high levels, with 3000-4000 ng/g dw in the surface sediments. The other methylphenols generally occur in the range 1-10 ng/g dw, except for 2-methylphenol that was never detectable. Of the long-chain alkylphenols, 4-NP and 4-NPEO1 are most abundant with levels in the range 75- 290 ng/g dw at the surface and higher at depth.

As an indication of urban influence, the levels at the upstream site were compared to the two central stations. 4-t-OP, 4-NP and their mono- and diethoxylates are consistently enriched by about a factor 2, suggesting a local impact. This is in agreement with a preceding study covering more sites in Stockholm (Sternbeck et al., 2003). The tertiary butylphenols and the methylphenols cannot be assessed in this respect, due to too few samples with detectable levels. Compared to the other sediments in this study, however, it appears that 4-methylphenol is in the same range as certain industrially affected sediments.

Most long-chain alkylphenols display lower levels at the surface compared to depth, suggesting that releases may have declined over time. 4-methylphenol is consistently higher at surface, which probably reflects degradation in sediments over time since 4-MP can be degraded also anaerobically (e.g. Heider & Fuchs, 1997, Spence et al., 2001).

12.4.2 Air

Five air samples were taken in fall 2003 in two major cities: Stockholm and Malmö. The most abundant substances were the methylphenols, which occurred in most samples and in fairly similar levels. Most tertiary butylphenols and long-chain alkylphenols were undetectable. The results are summarised in Table 30. From this limited dataset, an urban influence is only suggested for methylphenols, although levels are similar also in industrial areas. Higher levels have been detected in Swedish cities during strong influence of wood combustion (Table 13).

Road traffic is also a source of methylphenols, with 4-methylphenol dominating over 2- and 3-methylphenol by at least a factor of 4 (Kurtenbach et al., 2002). Methylphenols are also formed in the atmosphere through oxidation of toluene and xylene (major vehicle pollutants) why traffic may indirectly lead to formation of methylphenols. The ratio of 4-MP to 2-MP or 3-MP is consistently around 1 in our air samples, suggesting that direct emissions from road traffic is not the major source.

Table 30. Detectable compounds in urban air.

Compound	n > d.l. n _{max} = 5	Concentration range ng/m ³	Comment
4-t-butylphenol	3	0.1- 0.3	Similar levels in background and industrial areas
t-butylhydroquinone	2	0.05-0.08	Not detected in other areas
2,6-di-t-butylphenol	1	0.09	Occasionally found in industrial and background areas, at similar levels
2,6-di-t-butyl-4-methylphenol	5	0.08-0.43	Occasionally found in industrial and background areas, at similar levels
2-Methylphenol	4	1.4-3.9	Concentration range similar as in industrial areas; higher than in background areas
3-Methylphenol	5	2.4-4.1	
4-Methylphenol	5	1.5-5.2	Found in all industrial and background samples, at similar levels
2,4-Dimethylphenol	5	1.2-3.7	Concentration range similar as in industrial areas; higher than in background areas
3,4-Dimethylphenol	5	0.7-2.2	
4-nonylphenol (i.m.)	1	2.9	only found in one other air sample

Conclusively, air data suggest a moderate urban influence of methylphenols. Possible sources are wood combustion or oxidation of atmospheric toluene and xylene, rather than emissions from chemical use. The sediments indicate an urban influence on the levels of 4-t-OP, 4-NP and their mono- and diethoxylates, and also of 4-methylphenol. It cannot be ruled out that the origin of 4-methylphenol is natural (bacterial degradation of proteins) rather than anthropogenic. Thus, of all these substances, data only support that diffuse emissions occur for the long-chain alkylphenols.

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Appendix

Table A 1. List of samples, national sampling programme

Category	Sample #	Matrix	Site	Sampling date	Sampling date, end	X RT90	Y RT90	DW, %
Background	MR-3248	Air	Råö	2003-11-25	2013-12-09			
	MR-3249	Air	Råö	2003-12-15	2003-12-22			
	MR-3350	Fish	Fladen, herring P2002/1482-86	2002-09-10				
	MR-3351	Fish	Fladen, herring P2002/1487-91	2002-09-10				
	MR-3352	Fish	Fladen, herring P2002/1492-96	2002-09-10				
	MR-3320	Air	Pallas	2003-12-01	2003-12-17			
	MR-3322	Air	Pallas	2003-12-17	2003-12-31			
Urban & urban back-ground		Air	Stockholm, Hudiksvallsgatan 2	2003-10-20	2003-10-29			
		Air	Stockholm, Hudiksvallsgatan 2	2003-10-29	2003-11-13			
	MR-3314	Sediment	Stockholm, Essingen 0-2 cm	2003-12-20		6579212	1623633	18
	MR-3315	Sediment	Stockholm, Essingen 33-35 cm	2003-12-20		6579212	1623633	23
	MR-3316	Sediment	Stockholm, Riddarfjärden 0-2 cm	2003-12-20		6580105	1627283	13
	MR-3317	Sediment	Stockholm, Riddarfjärden 33-35 cm	2003-12-20		6580105	1627283	31
	MR-3318	Sediment	Stockholm, Årstaviken 0-2 cm	2003-12-20		6578147	1628321	19
	MR-3319	Sediment	Stockholm, Årstaviken 33-35 cm	2003-12-20		6578147	1628321	24
	MR-3262	Air	Malmö, Rådhuset	2003-10-28	2003-11-12			
	MR-3264	Air	Malmö, Rådhuset	2003-11-13	2003-11-26			
MR-3266	Air	Malmö, Rådhuset	2003-11-28	2003-12-12				
Paint industry	MR-3067	Air	Malmö, Anonymous	2003-10-28	2003-11-04			
	MR-3176	Air	Malmö, Anonymous	2003-11-11	2003-11-25			
	MR-3240	Air	Malmö, Anonymous	2003-11-25	2003-12-12			
	MR-3049	Sediment	River, upstream anonymous point source	2003-10-28				32
	MR-3060	Effluent Ind	Waste water, anonymous point source	2003-10-31				
	MR-3061	Effluent Ind	Waste water, anonymous point source	2003-10-31				
	MR-3062	Effluent Ind	Waste water, anonymous point source	2003-10-31				
	MR-3050	Sediment	River, downstream anonymous point source	2003-10-29				25
	MR-3051	Sediment	River, downstream anonymous point source	2003-10-29				26

Table A 2. Cont.

Category	Sample #	Matrix	Site	Sampling date	Sampling date, end	X RT90	Y RT90	DW, %
Potentially contaminated site	MR-3254	Air	Trollhättan	2003-12-01	2003-12-16			
	MR-3275	Air	Trollhättan	2003-12-16	2003-12-30			
	MR-3417	Sludge	Trollhättan, Arvidstorp STP					22
	MR-3418	Sludge	Trollhättan, Arvidstorp STP					20
	MR-3419	Sludge	Trollhättan, Arvidstorp STP					20
	MR-3353	Soil	Trollhättan, Stallbacka					83
	MR-3354	Soil	Trollhättan, Stallbacka					93
	MR-3355	Soil	Trollhättan, Stallbacka					93
Chemical industry, phenolic resin producer	MR-3117	Air	Perstorp	2003-10-29	2003-11-12			
	MR-3241	Air	Perstorp	2003-12-04	2003-12-12			
	MR-3047	Surface water	Ybbarpsjön, upstream Perstorp	2003-10-29		6225194	1350744	
	MR-3043 1(3)	Sediment	Ybbarpsjön 0-5 cm, upstream Perstorp	2003-10-29		6225194	1350744	2,9
	MR-3043 2(3)	Sediment	Ybbarpsjön 0-5 cm, upstream Perstorp	2003-10-29		6225194	1350744	4,8
	MR-3043 3(3)	Sediment	Ybbarpsjön 0-5 cm, upstream Perstorp	2003-10-29		6225194	1350744	3,6
	MR-3145	Effluent Ind	Perstorp, industrial WWTP	2003-10-30				
	MR-3146	Effluent Ind	Perstorp, industrial WWTP	2003-11-04				
	MR-3147	Effluent Ind	Perstorp, industrial WWTP	2003-11-07				
	MR-3046	Sludge Ind	Perstorp, industrial WWTP	2003-10-29				1,0
	MR-3184	Sludge Ind	Perstorp, industrial WWTP	2003-11-06				1,1
	MR-3185	Sludge Ind	Perstorp, industrial WWTP	2003-11-04				1,1
	MR-3048	Surface water	Storarydsdammen, downstream Perstorp	2003-10-29		6222203	1346655	
	MR-3044 1(3)	Sediment	Storarydsdammen 0-5 cm, downstream Perstorp	2003-10-29		6222203	1346655	4,3
	MR-3044 2(3)	Sediment	Storarydsdammen 0-5 cm, downstream Perstorp	2003-10-29		6222203	1346655	3,6
	MR-3044 3(3)	Sediment	Storarydsdammen 0-5 cm, downstream Perstorp	2003-10-29		6222203	1346655	4,2

Table A 3. List of samples, national sampling programme

Category	Sample #	Matrix	Site	Sampling date	Sampling date, end	X RT90	Y RT90	DW, %
Chemical/plastics industry	MR-3251	Air	Stenungsund	2003-11-25	2003-12-01			
	MR-3252	Air	Stenungsund	2003-12-03	2003-12-17			
	MR-2407	Sediment	200m from point source, site A5	2001 nov.				54
	MR-2409	Sediment	1000 m from point source, site E1	2001 nov.				44
	MR-3356	Sludge	Stenungsund, Stråvliden STP	2004-04-16				18
	MR-3357	Sludge	Stenungsund, Stråvliden STP	2004-04-16				18
	MR-3358	Sludge	Stenungsund, Stråvliden STP	2004-04-16				18
Household/consumption	MR-3324	Effluent	Vimmerby STP	2004-01-13				
	MR-3325	Effluent	Vimmerby STP	2004-01-14				
	MR-3326	Effluent	Vimmerby STP	2004-01-16				
	MR-3327	Sludge	Vimmerby STP	2004-01-13				23
	MR-3328	Sludge	Vimmerby STP	2004-01-14				23
	MR-3329	Sludge	Vimmerby STP	2004-01-16				23
	MR-3339	Effluent	Stockholm, Henriksdal STP	2004-02-08				
	MR-3340	Effluent	Stockholm, Henriksdal STP	2004-02-09				
	MR-3341	Effluent	Stockholm, Henriksdal STP	2004-02-10				
	MR-3342	Sludge	Stockholm, Henriksdal STP	2004-02-08				2,6
	MR-3343	sludge	Stockholm, Henriksdal STP	2004-02-09				2,6
	MR-3344	sludge	Stockholm, Henriksdal STP	2004-02-10				2,6

Table A 4. List of samples, county of Skåne

Sample #	Matrix	Site	Sampling date	X RT90	Y RT90	DW, %
MR-2934	Surface water	Lund, Vombsjön	2003-09-15			
MR-2951	Influent	Malmö, Sjölundaverket STP	2003-10-01			
MR-2936	Sludge	Malmö, Sjölundaverket STP	2003-09-17			2.9
MR-2937	Storm water	Malmö, SKA storm water	2003-09-17			
MR-2942	Influent	Trelleborg STP	2003-09-18			
MR-2948	Sludge	Trelleborg STP	2003-09-25			27
MR-2945	Sludge	Hässleholm STP	2003-09-18			0.5
MR-2944	Storm water	Hässleholm Maglekärnsbäck	2003-09-18			
MR-2949	Sludge	Ystad STP	2003-09-24			19
MR-2950	Storm water	Ystad	2003-09-26			
MR-2953	Influent	Landskrona, Lundåkraverket STP	2003-09-25			
MR-2952	Sludge	Landskrona, Lundåkraverket STP	2003-09-25			17
MR-3035	Influent	Bromölla STP	2003-10-15			
MR-3036	Sludge	Bromölla STP	2003-10-15			4,1
MR-2947	Sludge	Helsingborg, Öresundsverket STP	2003-09-23			24
MR-2971	Sediment	Helsingborg (coast / harbour)	2003-09-15			49
MR-2946	Storm water	Helsingborg, Ättekulla	2003-09-23			
MR-3055	Influent	Perstorp STP	2003-10-27			
MR-3053	Sludge	Perstorp STP	2003-10-27			18
MR-3054	Storm water	Perstorp	2003-10-27			
MR-2935	Sludge	Hörby STP	2003-09-16			13
MR-2970	Sludge	Svedala STP	2003-09-26			30
MR-2956	Fish, lake	Ivösjön (Bromölla, Kristianstad), perch	2003-09-24			
MR-2957	Fish, lake	Östra Ringsjön (Höör, Hörby), perch	2003-09-30			
MR-2961	Fish, lake	Västersjön/Rössjön (Ängelholm), perch	2003-09-25			
MR-2962	Fish, lake	Krageholmssjön (Ystad), perch	2003-09-22			
MR-2960	Fish, lake	Fjällfotasjön (Svedala), perch	2003-09-22			
MR-2958	Fish,lake	Storarydsdammen (Perstorp, Klippan), perch	2003-09-26			
MR-2959	Fish, lake	Store damm/Fåglasjön (Perstorp, Hässleholm), perch	2003-09-23			
MR-2955	Fish, lake	Finjasjön (Hässleholm), perch	2003-09-22			
MR-3038	Fish, coast	Spillepeng (Malmö), flounder	2003-09-22			
MR-2972	Fish, coast	Helsingborg (R3), flounder				

Table A 5. List of samples, county of Värmland

Sample #	Matrix	Site	Sampling date	X RT90	Y RT90	DW, %
MR-2938	Influent	Karlstad, Sjöstadverket STP	2003-09-18			
MR-2939	Sludge	Karlstad, Sjöstadverket STP	2003-09-18			25
MR-2954	Water	Skoghall, Akzo Nobel	2003-09-25			
MR-3192	Sediment	Skoghallsådran, Akzo Nobel	2003-11-26	6580520	136552	47
MR-3191	Sediment	Skoghall, Akzo Nobel, Anholms V	2003-11-26	6580710	1365360	45
MR-3193	Sediment	Skoghalls Bruk, Stora Enso	2003-11-26	6579430	1364930	42
MR-3194	Sediment	Grums, Billerud AB, Gruvöns bruk	2003-11-26	6582600	1347790	10
MR-2973	Sediment	Glafs fjorden, fiberbank	2003-10-09			19
MR-2969	Sludge	Kristinehamn, STP	2003-09-29			28
MR-2975	Sludge	Arvika, STP	2003-10-09			14

Table A 6. List of samples, county of Jönköping

Sample #	Matrix	Site	Sampling date	X RT90	Y RT90	DW %
MR-3057	Influent	Jönköping STP	2003-10-29			
MR-3056	Effluent	Jönköping STP	2003-10-29			
MR-3058	Sludge	Jönköping STP	2003-10-29			20
MR-3059	Sediment	Jönköping, Munksjön	2003-10-29			5.1
MR-3039	Influent	Gislaved STP	2003-10-22			
MR-3040	Effluent	Gislaved STP	2003-10-22			
MR-3041	Sludge	Gislaved STP	2003-10-21			18
MR-3037	Sediment	Gislaved	2003-10-15			48
MR-3198	Influent	Landsbro STP	2003-11-27			
MR-3197	Effluent	Landsbro STP	2003-11-27			
MR-3196	Sludge	Landsbro STP	2003-11-27			2.5
MR-3195	Sediment	Landsbro, Gröpplebäcken	2003-11-27			11
MR-3063	Influent	Hultsfred STP	2003-10-29			
MR-3064	Effluent	Hultsfred STP	2003-10-29			
MR-3065	Sludge	Hultsfred STP	2003-10-29			27
MR-3066	Sediment	Hultsfred, Hulingen	2003-10-29			19
MR-3336	Storm water	Vättern, Road traffic run off BHT 1	2004-02-09			
MR-3337	Storm water	Vättern, Road traffic run off BHT 2	2004-02-09			
MR-3338	Storm water	Vättern, Road traffic run off BHT 3	2004-02-09			

Table A 7. Concentrations of tertiary butylphenols and related substances in water.

Sample #	Prog.	Matrix	Site	Unit	2-tert-Butyl-phenol	4-tert-Butyl-phenol	2,6-Diiso-propyl-phenol	6-tert-Butyl-2,4-xylenol	tert-Butyl-4-hydroxy-anisole	2,4-Di-tert-butyl-phenol	Iso-eugenol	tert-Butyl-hydro-quinone	4-tert-Butyl-toluen	2,6-Di-tert-butyl-phenol	2,6-Di-iso-butyl-phenol	2,6-Di-tert-butyl-4-methyl-phenol	2,6-Di-tert-butyl-4-ethylphenol	2,4,6-Tri-tert-butylphenol
MR-2944	Skåne	SW	Hässleholm Maglekärnsbäck 03-09-18	µg/l	0.00077	0.0067	0.0017	<0.005	<0.002	0.015	<0.002	0.0028		0.00059	<0.02	<0.005	0.00042	0.00029
MR-2946	Skåne	SW	Helsingborg Ättekulla	µg/l	<0.002	0.014	<0.0009	<0.002	<0.002	0.044	<0.002	0.0063		0.00037	<0.01	<0.005	0.00015	0.00056
MR-2950	Skåne	SW	Ystad 03-09-26	µg/l	<0.001	0.0025	<0.00085	<0.002	<0.002	<0.001	<0.002	0.00091		0.00028	<0.02	<0.005	0.00014	0.00034
MR-2954	Värml	GW	Skoghäll Akzo Nobel groundwater 03-09-25	µg/l														
MR-3039	Jönk	Influent	Gislaved STP 03-10-21-22	µg/l	0.018	0.040	0.022	<0.04	0.03	0.035	<0.008	0.027	<0.0009	0.019	<0.1	2.71	<0.003	0.012
MR-3040	Jönk	Effluent	Gislaved STP 03-10-21-22	µg/l	0.0046	0.048	0.0063	<0.02	0.03	0.023	<0.001	0.014	<0.0005	0.0026	<0.01	0.094	0.0019	0.0016
MR-3057	Jönk	Influent	Jönköping STP 03-10-29	µg/l	<0.02	0.071	0.13	<0.008	0.12	2.16	<0.005	0.031	<0.0006	0.0040	<0.02	0.12	<0.0004	0.00044
MR-3056	Jönk	Effluent	Jönköping STP 03-10-29	µg/l	0.00075	0.013	0.00036	0.0011	0.00057	0.0074	0.00010	0.0011	<0.0004	0.00045	0.0015	0.10	<0.0003	0.000051
MR-3063	Jönk	Influent	Hultsfred STP 03-10-29	µg/l	0.014	0.038	0.016	<0.01	0.060	0.057	<0.006	<0.05	<0.0005	<0.0009	<0.03	0.15	0.00097	0.00047
MR-3064	Jönk	Effluent	Hultsfred STP 03-10-30	µg/l	0.00093	0.012	0.00060	0.0016	<0.002	0.013	<0.002	<0.002	<0.0004	0.00089	<0.006	<0.04	<0.0004	0.0013
MR-3198	Jönk	Influent	Landsbro STP 03-11-27	µg/l	0.011	0.10	0.037	0.012	0.14	0.45	0.019	0.040	<0.0004	0.0014	<0.02	0.10	0.0010	0.00036
MR-3197	Jönk	Effluent	Landsbro STP 03-11-27	µg/l	0.0045	0.033	0.010	<0.006	0.0029	0.065	<0.002	0.0075	<0.0009	<0.0006	<0.02	<0.04	<0.0006	<0.0003
MR-3324	nat	Effluent	Vimmerby STP 040113	µg/l	0.0036	0.015	0.0036	0.0020	0.0034	0.024	<0.001	0.0051	<0.0006	0.0030	<0.01	<0.03	0.0018	0.00065
MR-3325	nat	Effluent	Vimmerby STP 040114	µg/l	0.0040	0.016	0.0023	0.0024	0.0028	0.018	<0.001	0.0040	<0.0009	0.0012	<0.01	<0.03	0.00040	<0.0002
MR-3326	nat	Effluent	Vimmerby STP 040116	µg/l	0.0037	0.023	0.0016	0.0041	0.0026	0.016	<0.001	0.0046	<0.0005	0.00079	<0.01	<0.03	0.00020	<0.0001
MR-3339	nat	Effluent	Stockholm, Henriksdal STP 04-02-08	µg/l	0.0028	0.0067	0.0051	0.0013	0.0027	0.015	<0.001	0.0046	<0.0006	0.00049	<0.01	<0.006	<0.0004	<0.0001
MR-3340	nat	Effluent	Stockholm, Henriksdal STP 04-02-09	µg/l	0.0028	0.0059	0.0072	<0.003	<0.002	0.013	<0.002	0.0040	<0.009	0.0038	<0.02	<0.09	<0.006	<0.002
MR-3341	nat	Effluent	Stockholm, Henriksdal STP 04-02-10	µg/l	0.0028	0.0061	0.011	<0.004	<0.003	0.013	<0.002	0.0048	<0.009	<0.006	<0.02	<0.07	<0.006	<0.002
MR-3047	nat	W	Ybbarpsjön, upstream Perstorp	µg/l	0.00019	0.00035		0.00013	0.00016	0.015	0.00037		<0.0006	<0.0004	0.0026	<0.02	<0.0003	0.000071
MR-3048	nat	W	Storarydsdammen, downstream Perstorp	µg/l	<0.002	<0.003	0.00033	<0.002	<0.001	0.020	<0.001	<0.0007	<0.0004	0.00039	<0.009	<0.01	0.000033	0.000033
MR-3145	nat	Effluent Ind	Perstorp daily sample	µg/l	<0.005	0.0032	0.0033	0.0016	0.0009	0.039	<0.002	<0.001	<0.0005	0.0013	0.0014	<0.02	<0.0003	<0.0001
MR-3146	nat	Effluent Ind	Perstorp daily sample	µg/l	0.0016	0.013	0.0063	0.0038	<0.002	0.17	<0.002	<0.001	<0.0005	0.0027	<0.02	<0.01	0.0013	0.00023
MR-3147	nat	Effluent Ind	Perstorp daily sample	µg/l	0.0017	0.0098	<0.0006	<0.002	<0.001	0.11	<0.001	0.00025	<0.0004	<0.0003	<0.010	<0.02	<0.0003	<0.0001
MR-3054	Skåne	SW	Perstorp 03-10-27	µg/l	0.00022	0.0021	0.000089	0.00070	0.00020	0.047	0.00037	0.00066		0.00019	0.0034	<0.02	0.000055	<0.0002
MR-3055	Skåne	Influent	Perstorp STP 03-10-27	µg/l	0.0030	0.028	0.029	0.018	0.044	0.11	0.0033	0.0034		0.016	<0.02	0.33	0.0010	0.0020
MR-3060	nat	Effluent Ind	Malmö, Anonymous	µg/l	0.0029	0.044	0.00048	0.028	<0.003	0.041	<0.002	<0.01	<0.0003	0.0030	<0.02	0.22	0.00015	0.00078
MR-3061	nat	Effluent Ind	Malmö, Anonymous	µg/l	0.0037	0.063	0.0010	0.037	<0.01	0.045	<0.002	<0.01	<0.0003	0.0018	<0.01	0.44	<0.0004	0.00027
MR-3062	nat	Effluent Ind	Malmö, Anonymous	µg/l	<0.006	0.075	<0.002	0.041	0.035	0.045	<0.004	<0.003	<0.0004	0.0015	<0.02	0.083	<0.0002	<0.0001
MR-2934	Skåne	W	Malmö, Vombsjön	µg/l	<0.001	<0.001	<0.001	<0.002	<0.002	0.0068	<0.002	0.0026		0.00020	<0.01	<0.005	0.00010	0.00022
MR-2937	Skåne	SW	Malmö SKA Storm Water	µg/l	<0.001	0.0038	<0.0009	0.0053	<0.003	0.12	<0.002	0.0063		0.00037	<0.02	<0.005	0.00029	0.00047
MR-2951	Skåne	Influent	Malmö, Sjölundaverket STP 03-10-01	µg/l	0.016	0.14	0.041	<0.005	0.15	0.097	0.42	0.073		0.012	<0.02	0.53	0.00052	0.00536

Table A 7. Cont.

Sample #	Prog.	Matrix	Site	Unit	2-tert-Butyl-phenol	4-tert-Butyl-phenol	2,6-Diisopropyl-phenol	6-tert-Butyl-2,4-xyleneol	tert-Butyl-4-hydroxy-anisole	2,4-Di-tert-butyl-phenol	Iso-eugenol	tert-Butyl-hydro-quinone	4-tert-Butyl-toluen	2,6-Di-tert-butyl-phenol	2,6-Di-iso-butyl-phenol	2,6-Di-tert-butyl-4-methyl-phenol	2,6-Di-tert-butyl-4-ethylphenol	2,4,6-Tri-tert-butylphenol
MR-2938	Värml	Influent	Karlstad Sjöstadsverket STP 03-09-18	µg/l	<0.03	<0.04	0.22	<0.04	0.17	0.046	0.047	0.079	<0.001	0.021	<0.06	0.56	0.0074	0.0059
MR-2942	Skåne	Influent	Trelleborg STP 03-09-18	µg/l	0.025	1.89	0.19	<0.006	0.29	0.083	0.12	0.020		0.0036	<0.02	0.19	0.00054	0.00087
MR-2953	Skåne	Influent	Landskrona, Lundåkraverket STP	µg/l	0.0086	0.080	0.050	<0.006	0.15	0.042	<0.007	0.017		0.0026	<0.02	0.28	0.0010	<0.001
MR-3035	Skåne	Influent	Bromölla STP 03-10-15	µg/l	0.030	0.064	0.0092	<0.01	0.13	0.13	0.0050	<0.001		0.0080	<0.01	0.59	0.0051	0.0027
MR-3336	Jönk	SW	Vättern, Road traffic runoff BHT 1	µg/l	<0.003	0.048	<0.001	<0.003	<0.003	0.058	<0.003	<0.004	<0.0004	0.00098	<0.04	<0.003	<0.0003	0.000090
MR-3337	Jönk	SW	Vättern, Road traffic runoff BHT 2	µg/l	<0.002	0.047	<0.002	<0.005	<0.002	0.065	<0.003	<0.002	<0.0004	0.0019	<0.03	<0.003	<0.0002	<0.00008
MR-3338	Jönk	SW	Vättern, Road traffic runoff BHT 3	µg/l	<0.0003	0.062	<0.001	0.0041	<0.004	0.099	<0.004	<0.003	<0.0004	0.0023	<0.04	<0.003	<0.0003	0.000047

Table A 8. Concentration of methylphenols and long-chained alkylphenols in water.

Sample #	Prog.	Matrix	Site	Unit	2-Methyl-phenol	3-Methyl-phenol	4-Methyl-phenol	2,4-Di-methyl-phenol	3,5-Di-methyl-phenol	2,3-Di-methyl-phenol	3,4-Di-methyl-phenol	4-n-OP	4-t-OP	4-t-OP-EO1	4-t-OP-EO2	4-n-NP	4-NP	4-NP-EO1	4-NP-EO2	4-DP
MR-2944	Skåne	SW	Hässleholm Maglekärrsbäck 03-09-18	µg/l									0.0070	0.0098	0.0032	<0.001	0.26	0.077	<0.01	<0.01
MR-2946	Skåne	SW	Helsingborg Ättekulla	µg/l								<0.002	0.011	<0.004	0.0056	<0.005	0.18		0.063	<0.005
MR-2950	Skåne	SW	Ystad 03-09-26	µg/l								<0.002	0.0029	0.0023	0.0011	0.0020	0.047	<0.1	<0.03	<0.004
MR-2954	Värml	GrW	Skoghall Akzo Nobel groundwater 03-09-25	µg/l	11	45	33	35	15	5.9	5.2									
MR-3039	Jönk	Influent	Gislaved STP 03-10-21-22	µg/l																
MR-3040	Jönk	Effluent	Gislaved STP 03-10-21-22	µg/l																
MR-3057	Jönk	Influent	Jönköping STP 03-10-29	µg/l	0.13	0.17	40	0.20		0.65	0.029									
MR-3056	Jönk	Effluent	Jönköping STP03-10-29	µg/l	0.016	0.0033	0.023	<0.003	<0.002	<0.002	<0.003									
MR-3063	Jönk	Influent	Hultsfred STP 03-10-29	µg/l																
MR-3064	Jönk	Effluent	Hultsfred STP 03-10-30	µg/l																
MR-3198	Jönk	Influent	Landsbro STP 03-11-27	µg/l	0.12	0.023	44	0.11	<0.06	<0.09	0.010									
MR-3197	Jönk	Effluent	Landsbro STP 03-11-27	µg/l	0.020	0.0046	0.028	0.011	0.0015	0.0032	0.0020									
MR-3324	nat	Effluent	Vimmerby STP 040113	µg/l	0.0090	0.0052	0.018	0.0094	0.0020	0.0033	0.0031	<0.002	0.032	<0.002	0.0023	0.011	0.19	0.081	0.02	<0.003
MR-3325	nat	Effluent	Vimmerby STP 040114	µg/l	0.010	0.013	0.020	0.013	0.0023	0.0052	0.0039	<0.002	0.036	<0.002	0.0025	0.0066	1.0	0.12	0.02	<0.003
MR-3326	nat	Effluent	Vimmerby STP 040116	µg/l	0.010	0.0082	0.030	0.017	0.0018	0.0047	0.0032	<0.002	0.035	<0.004	0.0026	0.0027	0.40	0.12	0.03	<0.004
MR-3339	nat	Effluent	Stockholm, Henriksdal STP 04-02-08.	µg/l	0.019	0.0042	0.014	0.0051	0.0052	0.0012	0.0025	<0.002	0.011	0.0029	0.0021	<0.003	0.11	0.075	0.0089	<0.005
MR-3340	nat	Effluent	Stockholm, Henriksdal STP 04-02-09.	µg/l	0.013	0.0028	0.013	0.0054	0.0037	0.0019	0.0019	<0.002	0.0076	<0.0003	0.0012	<0.003	0.095	0.060	<0.02	<0.004
MR-3341	nat	Effluent	Stockholm, Henriksdal STP 04-02-10	µg/l	0.014	0.0026	0.012	0.0048	0.0040	0.0020	0.0013	<0.002	0.0051	0.0022	0.00093	<0.002	0.028	0.050	0.0082	<0.003
MR-3047	nat	W	Ybbarpsjön, upstream Perstorp	µg/l	0.0037	0.0012	0.0092	0.0026	0.0052	0.0012	0.0012	<0.002	0.0030	0.00050	<0.002	0.00044	0.033	<0.01	<0.04	<0.006
MR-3048	nat	W	Storarydsdammen, downstream Perstorp	µg/l	0.027	0.014	0.015	0.077	0.059	0.010	0.012	<0.002	0.0056	<0.0006	<0.0008	<0.0005	0.32	<0.05	<0.01	<0.004
MR-3145	nat	Effluent Ind	Perstorp daily sample	µg/l	<0.005	<0.005	0.015	0.024	0.0017	0.0035	0.0050	<0.002	0.012	0.00040	<0.002	0.0034	0.20	<0.01	<0.05	<0.007
MR-3146	nat	Effluent Ind	Perstorp daily sample	µg/l	0.0045	0.0016	0.018	0.0068	<0.002	<0.003	<0.003	<0.002	0.019	<0.0009	<0.001	0.034	0.17	0.003	<0.03	
MR-3147	nat	Effluent Ind	Perstorp daily sample	µg/l	<0.002	<0.002	0.0066	0.0092	0.0014	0.0012	0.0013	<0.002	0.013	<0.0006		0.010	0.24	0.01	<0.02	
MR-3054	Skåne	SW	Perstorp	µg/l								<0.002	0.0065	0.0019	<0.0007	<0.0007	0.078	0.022	<0.02	<0.002
MR-3055	Skåne	Influent	Perstorp STP	µg/l									0.070	0.096	0.006	0.071	3.4	1.1	0.05	<0.1
MR-3060	nat	Effluent Ind	Malmö, Anonymous	µg/l	0.078	0.067	6.8	0.062	<0.006	<0.04	<0.02	<0.002	0.22	<0.04	<0.003	<0.005	5.5	<0.04	<0.05	<0.02
MR-3061	nat	Effluent Ind	Malmö, Anonymous	µg/l	0.14	0.084	15	<0.3	<0.1	<0.1	0.065	<0.002	0.12	0.027	0.01	<0.01	4.1	2.5	0.12	<0.04
MR-3062	nat	Effluent Ind	Malmö, Anonymous	µg/l	0.16	0.11	14	0.18	<0.06	<0.07	0.076	<0.002	0.12	0.056	<0.007	0.067	3.5	1.8	<0.4	<0.06
MR-2934	Skåne	W	Malmö, Vombsjön	µg/l								<0.002	0.0036	0.0067	0.0026	0.0052	0.27	0.057	<0.02	<0.004
MR-2937	Skåne	SW	Malmö SKA Storm Water	µg/l								<0.002	0.016	0.015	0.0039	<0.002	0.092	0.19	<0.02	<0.01
MR-2951	Skåne	Influent	Malmö, Sjölundaverket STP 03-10-01	µg/l								<0.002	0.052		0.089	<0.002	1.2	<5.3	<1.0	<0.02
MR-2938	Värml	Influent	Karlstad Sjöstadsverket STP 03-09-18	µg/l	0.31	0.16	58	0.24	0.72	0.81	<0.04	<0.002	0.066	<2.3	<0.01	0.018	1.7	<1.0	0.29	<0.06
MR-2942	Skåne	Influent	Trelleborg STP 03-09-18	µg/l									0.086	<1.7	0.044		1.7	<5.8	<0.6	<0.04
MR-2953	Skåne	Influent	Landskrona, Lundåkraverket STP	µg/l								<0.002	0.16		0.12	0.012	0.99	1.03	0.077	<0.06
MR-3035	Skåne	Influent	Bromölla STP 03-10-15	µg/l								<0.002	0.030	0.057	<0.02	<0.1	1.2	0.89	0.17	<0.1
MR-3336	Jönk	SW	Vättern, Road traffic runoff BHT 1	µg/l																
MR-3337	Jönk	SW	Vättern, Road traffic runoff BHT 2	µg/l																
MR-3338	Jönk	SW	Vättern, Road traffic runoff BHT 3	µg/l																

Table A 9. Concentration of tert butylphenols in sewage sludge.

Sample #	Prog.	Matrix	Site	Unit	2-tert-Butyl-phenol	4-tert-Butyl-phenol	2,6-Diisopropyl-phenol	6-tert-Butyl-2,4-xyleneol	tert-Butyl-4-hydroxy-anisole	2,4-Di-tert-butyl-phenol	Iso-eugenol	tert-Butyl-hydroquinone	4-tert-Butyl-toluen	2,6-Di-tert-butyl-phenol	2,6-Di-isobutyl-phenol	2,6-Di-tert-butyl-4-methyl-phenol	2,6-Di-tert-butyl-4-ethylphenol	2,4,6-Tri-tert-butyl-phenol
MR-3046	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	<0.02	0.073	<0.01	<0.05	<0.04	0.024	<0.03	<0.03	<0.003	<0.002	<0.2	0.0030	<0.002	0.0020
MR-3184	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	0.020	0.057	0.038	0.091	0.071	0.13	<0.03	0.11	<0.02	<0.02	<0.1	0.014	<0.02	0.023
MR-3185	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	<0.006	0.015	<0.002	<0.01	<0.004	0.0070	<0.005	<0.01	<0.004	<0.003	<0.03	0.0020	<0.003	0.0010
MR-3053	Skåne	Sludge	Perstorp STP	µg/g DW	0.0040	0.016	0.0050	<0.01	<0.003	0.092	<0.003	<0.01		0.013	<0.02	1.7	0.0010	0.0020
MR-3327	nat	Sludge	Vimmerby STP	µg/g DW	0.0050	0.017	<0.001	<0.02	<0.001	<0.001	<0.002	0.0040	<0.003	<0.003	<0.02	0.017	<0.001	<0.0005
MR-3328	nat	Sludge	Vimmerby STP	µg/g DW	0.0060	0.014	0.0010	<0.03	<0.001	<0.001	<0.001	<0.001	<0.003	<0.002	<0.02	0.010	<0.0005	0.00017
MR-3329	nat	Sludge	Vimmerby STP	µg/g DW	0.0060	0.015	0.0010	<0.03	<0.001	<0.001	<0.002	<0.002	<0.005	<0.003	<0.02	0.0080	<0.001	<0.0004
MR-3356	nat	Sludge	Stenungsund, Stråvliden STP	µg/g DW	0.0030	0.0070	0.0020	<0.005	<0.003	0.11	<0.005	0.0050	<0.002	0.0020	<0.03	0.031	<0.001	0.00033
MR-3357	nat	Sludge	Stenungsund, Stråvliden STP	µg/g DW	0.0030	0.0050	0.0010	<0.003	<0.003	0.12	0.010	0.0060	<0.002	<0.002	<0.01	0.0050	<0.001	<0.001
MR-3358	nat	Sludge	Stenungsund, Stråvliden STP	µg/g DW	0.0030	0.0050	0.0010	<0.004	<0.003	0.11	<0.003	0.0070	<0.003	<0.002	<0.02	0.013	<0.001	<0.001
MR-3417	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	<0.006	0.012	0.035	<0.01	<0.004	0.12	<0.001	<0.01	<0.001	0.084	<0.02	0.93	<0.001	0.0034
MR-3418	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	<0.005	0.012	0.042	<0.02	<0.008	0.13	<0.007	<0.01	<0.001	0.095	<0.03	1.1	<0.001	0.0032
MR-3419	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	<0.005	0.013	0.040	<0.02	<0.008	0.13	<0.008	<0.01	<0.001	0.11	<0.01	1.2	<0.001	0.0037
MR-3342	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.001	0.029	0.0010	<0.03	<0.004	<0.004	<0.002	<0.01	<0.002	<0.003	<0.06	0.013	<0.001	<0.001
MR-3343	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.001	0.024	0.0010	<0.04	<0.002	<0.002	<0.003	<0.004	<0.003	<0.01	<0.03	0.019	<0.001	<0.001
MR-3344	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.001	0.026	<0.001	<0.04	<0.002	<0.002	<0.004	<0.01	<0.002	<0.01	<0.04	0.016	<0.002	<0.001
MR-2949	Skåne	Sludge	Ystad STP	µg/g DW	0.0040	0.10	0.043	<0.01	<0.003	37	<0.005	0.016		0.030	0.25	1.4	0.0030	0.011
MR-2948	Skåne	Sludge	Trelleborg STP	µg/g DW	0.0070	0.031	0.036	0.023	<0.002	0.11	<0.003	0.010		0.0050	<0.02	1.3	0.0010	0.0020
MR-2936	Skåne	Sludge	Malmö, Sjölundaverket STP	µg/g DW	0.0050	0.060	0.030	<0.006	<0.003	0.14	<0.01	<0.01		0.014	<0.03	0.44	0.00044	0.0030
MR-2970	Skåne	Sludge	Svedala STP	µg/g DW	0.0050	0.033	0.0020	0.010	<0.003	0.084	<0.001	0.0060		<0.0005	<0.02	<0.001	<0.0003	<0.0002
MR-2935	Skåne	Sludge	Hörby STP	µg/g DW	<0.001	<0.003	<0.001	<0.009	<0.003	0.029	<0.004	<0.005		<0.001	<0.02	0.011	<0.001	<0.0003
MR-3036	Skåne	Sludge	Bromölla STP	µg/g DW	0.0030	0.0090	0.0050	<0.01	0.040	0.10	<0.01	<0.01		0.0030	<0.03	1.0	0.0010	0.0010
MR-2952	Skåne	Sludge	Landskrona, Lundåkraverket STP	µg/g DW	0.0040	0.014	0.032	<0.01	0.0030	0.11	<0.003	<0.005		0.0060	<0.02	0.16	0.0010	0.0010
MR-2947	Skåne	Sludge	Helsingborg, Öresundsverket STP	µg/g DW	0.049	0.12	<0.02	<0.09	<0.04	3.5	<0.06	2.8		<0.04	<0.3	1.3	0.0070	0.018
MR-2945	Skåne	Sludge	Hässleholm STP	µg/g DW	<0.005	0.056	<0.004	<0.02	<0.01	0.013	<0.01	<0.01		<0.01	<0.07	<0.01	<0.01	<0.002
MR-3041	Jönköping	Sludge	Gislaved STP	µg/g DW	0.016	0.076	0.017	<0.02	0.028	0.45	<0.01	<0.05	0.0050	0.027	<0.1	0.96	0.0020	0.0080
MR-3065	Jönköping	Sludge	Hultsfred STP	µg/g DW	<0.0003	<0.001	<0.0002	<0.002	<0.0005	<0.0004	<0.0004	<0.001	<0.0003	<0.0002	<0.005	0.00018	<0.0002	<0.0001
MR-3196	Jönköping	Sludge	Landsbro STP	µg/g DW	0.0020	0.0080	<0.003	<0.004	<0.02	0.093	<0.004	0.021	<0.003	<0.002	<0.03	0.21	<0.002	0.00029
MR-3058	Jönköping	Sludge	Jönköping STP	µg/g DW	0.0030	0.012	0.036	<0.012	<0.003	0.15	<0.002	<0.01	0.0010	0.067	<0.03	0.06	<0.001	0.0010
MR-2939	Värmland	Sludge	Karlstad, Sjöstadsverket STP	µg/g DW	0.0050	0.042	0.063	<0.01	<0.002	0.16	<0.001	0.041	<0.001	0.023	<0.01	0.17	<0.001	0.0010
MR-2969	Värmland	Sludge	Kristinehamn, STP	µg/g DW	0.043	0.21	0.054	0.19	<0.02	1.2	<0.02	<0.01	0.017	0.19	<0.2	3.1	<0.02	0.15
MR-2975	Värmland	Sludge	Arvika, STP	µg/g DW	0.0080	0.037	0.044	<0.04	<0.002	0.18	<0.002	0.017	<0.005	0.24	<0.02	1.0	<0.001	0.0080

Screening tertiary butylphenols, methylphenols, and long-chain alkylphenols in the Swedish environment

IVL Rapport B1594

Table A 10. Concentration of methylphenols and long-chain alkylphenols in sewage sludge.

Sample #	Prog.	Matrix	Site	Unit	2-Methyl-phenol	3-Methyl-phenol	4-Methyl-phenol	2,4-Di-methyl-phenol	3,5-Di-methyl-phenol	2,3-Di-methyl-phenol	3,4-Di-methyl-phenol	4-n-OP	4-t-OP	4-t-OP-EO1	4-t-OP-EO2	4-n-NP	4-NP	4-NP-EO1	4-NP-EO2	4-DP
MR-3046	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	<0.05	<0.04	1396	<0.1	<0.03	<0.04	<0.04	<0.01	0.22		<0.05	6.3	8.1	4.2	<1.0	
MR-3184	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	<0.05	<0.05	845	<0.05	<0.04	<0.05	<0.05	<0.002	0.60	<0.05	0.12	8.2	8.6	0.80	<0.5	
MR-3185	nat	Sludge Ind	Perstorp, industrial WWTP	µg/g DW	<0.02	<0.03	524	<0.02	<0.01	<0.02	<0.02	<0.001	0.13	<0.07	<0.02	3.9	1.6	0.44	<0.2	
MR-3053	Skåne	Sludge	Perstorp STP	µg/g DW								0.0010	0.34	<0.18	<0.02	0.01	92	7.3	0.32	<0.1
MR-3327	nat	Sludge	Vimmerby STP	µg/g DW	<0.02	<0.005	0.076	<0.01	<0.002	<0.002	<0.01	0.0010	0.41	<0.01	0.01	16	9.3	0.45	<0.01	
MR-3328	nat	Sludge	Vimmerby STP	µg/g DW	<0.01	<0.003	0.056	<0.01	<0.002	<0.005	<0.004	0.0010	0.44	<0.1	0.0040	17	8.0	0.27	<0.02	
MR-3329	nat	Sludge	Vimmerby STP	µg/g DW	<0.02	<0.003	0.081	<0.005	<0.002	<0.003	<0.004	0.0010	0.49	<0.07	0.0030	19	8.2	0.20	<0.02	
MR-3356	nat	Sludge	Stenungsund, Strävlieden STP	µg/g DW	0.0070	<0.01	0.054	0.018	<0.01	<0.01	<0.01	<0.001	0.082	<0.02	0.02	1.7	3.0	0.60	<0.07	
MR-3357	nat	Sludge	Stenungsund, Strävlieden STP	µg/g DW	0.021	0.0040	0.081	0.020	<0.004	<0.004	<0.003	<0.001	0.094		0.02	2.0	3.2	0.60	0.045	
MR-3358	nat	Sludge	Stenungsund, Strävlieden STP	µg/g DW	0.0070	0.0040	0.15	0.022	<0.003	<0.004	<0.01	0.0010	0.076	<0.02	0.01	1.7	3.1	0.53	<0.08	
MR-3417	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	0.061	0.015	0.20	<0.02	<0.003	0.0088	<0.004	<0.004	0.45	<0.2	0.015	19	12	0.18	<0.04	
MR-3418	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	0.21	0.030	0.19	<0.01	<0.003	0.020	<0.003	<0.006	0.44	<0.2	0.019	18	9.1	0.21	<0.04	
MR-3419	nat	Sludge	Trollhättan, Arvidstorp STP	µg/g DW	0.034	0.046	0.23	<0.01	<0.003	0.019	<0.004	<0.006	0.47	<0.2	0.017	19	10	0.21	<0.04	
MR-3342	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.04	<0.01	0.13	<0.02	0.24	<0.02	<0.02	0.0010	0.86	<0.09	0.0050	24	4.5	0.19	<0.04	
MR-3343	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.03	<0.02	0.20	<0.01	0.28	<0.02	<0.005	0.0010	0.58	<0.2	0.0060	16	3.0	0.21	<0.02	
MR-3344	nat	Sludge	Stockholm, Henriksdal STP	µg/g DW	<0.04	<0.01	0.065	<0.01	0.27	<0.02	<0.02	0.0010	0.68	<0.2	0.0060	19	3.3	0.20	<0.03	
MR-2949	Skåne	Sludge	Ystad STP	µg/g DW								0.0010	0.80	<0.2	0.01	57	8.9	0.37	<0.07	
MR-2948	Skåne	Sludge	Trelleborg STP	µg/g DW								<0.001	0.64	<0.1	<0.01	30	6.8	0.26	<0.05	
MR-2936	Skåne	Sludge	Malmö, Sjölundaverket STP	µg/g DW								<0.002	0.97	<0.2	<0.02	36	12	0.37	<0.05	
MR-2970	Skåne	Sludge	Svedala STP	µg/g DW								<0.0003	0.20	0.53	0.15	4.0	8.2	5.2	<0.06	
MR-2935	Skåne	Sludge	Hörby STP	µg/g DW								<0.001	0.12		0.04	0.06	2.3	2.5	0.45	0.15
MR-3036	Skåne	Sludge	Bromölla STP	µg/g DW								<0.0004	0.14	0.31	0.02	0.04	4.6	17	0.72	0.030
MR-2952	Skåne	Sludge	Landskrona, Lundåkraverket STP	µg/g DW								0.0010	0.66		0.05	15	2.6	0.47	0.053	
MR-2947	Skåne	Sludge	Helsingborg, Öresundsverket STP	µg/g DW								<0.01	8.7	5.0	0.54	0.32	207	160	18	<2.1
MR-2945	Skåne	Sludge	Hässleholm STP	µg/g DW								0.0010	0.17	0.17	<0.02	<0.01	6.1	1.6	<0.4	<0.09
MR-3041	Jönköping	Sludge	Gislaved STP	µg/g DW																
MR-3065	Jönköping	Sludge	Hultsfred STP	µg/g DW																
MR-3196	Jönköping	Sludge	Landsbro STP	µg/g DW	0.077	0.0070	24	<0.03	<0.01	<0.02	<0.01									
MR-3058	Jönköping	Sludge	Jönköping STP	µg/g DW	0.0040	0.0040	0.65	<0.01	<0.01	<0.02	<0.005									
MR-2939	Värmland	Sludge	Karlstad, Sjöstadsverket STP	µg/g DW																
MR-2969	Värmland	Sludge	Kristinehamn, STP	µg/g DW								<0.004	7.1	0.32	0.12	0.094	437	59	5.1	1.4
MR-2975	Värmland	Sludge	Arvika, STP	µg/g DW	<0.013	<0.012	0.15	<0.007	0.076	0.022	0.0090	0.0030	0.76	0.43	<0.01	<0.6	28	19	0.54	<0.2

Table A 11. Concentration of tert butylphenols in sediment.

Sample #	Prog.	Matrix	Site	Unit	2-t-Butyl-phenol	4-t-Butyl-phenol	2,6-Diisopropyl-phenol	6-t-Butyl-2,4-xylene	t-Butyl-4-hydroxy-anisole	2,4-Di-t-butyl-phenol	Iso-eugenol	t-Butyl-hydro-quinone	4-t-Butyl-toluen	2,6-Di-t-butyl-phenol	2,6-Di-iso-butyl-phenol	2,6-Di-t-butyl-4-methyl-phenol	2,6-Di-t-butyl-4-ethyl-phenol	2,4,6-Tri-t-butyl-phenol
MR-3043 (1)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<1	<1	<0.8	<2	<2	<2	<2	<2	<2	<2	<19	<2	<2	<1
MR-3043 (2)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<1	<1	<0.5	<1	<2	<1	<3	<2	<1	<0.9	<12	<0.9	<0.8	<0.6
MR-3043 (3)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<2	<3	<2	<4	<6	<3	<13	3.5	<2	<1	<36	<1	<1	<0.8
MR-3044 (1)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	0.77	18	0.60	3.3	0.78	5.5	7.6	2.7	<0.4	<0.03	<12	1.5	<0.3	0.15
MR-3044 (2)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	1.4	15	0.54	3.0	2.9	3.4	14	2.6	<0.5	<0.3	<12	<0.9	<0.5	0.07
MR-3044 (3)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	1.3	28	0.30	1.3	0.73	6.3	16	2.5	<0.5	1.2	<11	2.1	<0.4	0.23
MR-2407	nat	Sed., ChemInd -coast	200m from point source, site A5	ng/g DW	<0.09	<0.06	<0.07	<0.2	<0.1	<0.5	<0.2	<0.2	<0.1	<0.09	<2	0.13	<0.05	<0.02
MR-2409	nat	Sed., ChemInd -coast	1000 m from point source, site E1	ng/g DW	<0.2	<0.08	<0.07	<0.2	0.71	0.7	0.76	<0.2	<0.2	<0.1	<2	0.24	<0.1	<0.03
MR-3049	nat	Sed., Backgr.	River, upstream anonymous point source	ng/g DW	<0.3	<0.2	<0.2	<1	<0.3	0.63	<0.3	<0.3	<0.07	<0.05	<2	0.10	<0.05	<0.02
MR-3050	nat	Sed., ChemInd	River, downstream anonymous point source	ng/g DW	<0.4	2.4	<0.1	<2	<1	5.2	<1	<0.5	<0.2	1.1	<3	<13	0.08	2.7
MR-3051	nat	Sed., ChemInd	River, downstream anonymous point source	ng/g DW	<0.4	3.1	<0.1	<2	<0.7	5.6	<0.5	1.0	<0.2	1.5	<2	<13	<0.1	3.5
MR-3191	Värmland	Sed., ChemInd	Skoghall, Akzo Nobel, Anholms V	ng/g DW														
MR-3192	Värmland	Sed., ChemInd	Skoghallsådran, Akzo Nobel	ng/g DW														
MR-3193	Värmland	Sed., PaperInd	Skoghalls Bruk, Stora Enso	ng/g DW														
MR-3194	Värmland	Sed., PaperInd	Grums, Billerud AB, Gruvöns bruk	ng/g DW														
MR-2973	Värmland	Sed., PaperInd	Glafs fjorden, fiberbank	ng/g DW	12	5.8	0.31	<11	0.74	23	6.0	2.2	<3	<2	<12	<1	<0.5	0.45
MR-3314	nat	Sed., Urban	Stockholm, Essingen 0-2 cm	ng/g DW	<0.2	<0.2	<0.2	<0.8	<0.8	<0.5	<0.8	<0.3	<0.2	<0.1	<3	<0.2	<0.2	0.02
MR-3315	nat	Sed., Urban	Stockholm, Essingen 33-35 cm	ng/g DW	<0.2	1.6	<0.1	<0.8	<0.8	<0.3	<0.81	<0.3	0.13	<0.4	<3	3.7	<0.2	0.01
MR-3316	nat	Sed., Urban	Stockholm, Riddarfjärden 0-2 cm	ng/g DW	0.20	10	0.59	0.83	0.83	2.5	1.7	0.45	<0.2	<0.3	<5	0.46	<0.2	0.04
MR-3317	nat	Sed., Urban	Stockholm, Riddarfjärden 33-35 cm	ng/g DW	<0.2	4.5	<0.1	<0.3	<0.3	<0.4	<2	0.62	0.60	<0.5	<3	<0.9	<0.5	<0.02
MR-3318	nat	Sed., Urban	Stockholm, Årstaviken 0-2 cm	ng/g DW	<0.2	1.5	<0.1	<0.3	<0.3	0.49	0.84	1.5	<0.2	<0.3	<3	<0.2	<0.1	0.03
MR-3319	nat	Sed., Urban	Stockholm, Årstaviken 33-35 cm	ng/g DW	<0.2	3.7	0.29	<0.6	<0.6	<0.5	<1	<0.4	0.17	<2	<3	1.8	<0.3	0.05
MR-3059	Jönköping	Sed., Urban	Jönköping, Munksjön	ng/g DW	<2	6.8	2.4	<7	<3	16	6.0	6.2	<1	<0.7	<16	<9	<0.7	0.06
MR-3037	Jönköping	Sed., STP rec	Gislaved	ng/g DW	<0.1	<0.1	<0.1	<0.4	<0.2	<0.5	<0.3	<0.3	<0.2	<0.1	<2	0.84	<0.1	0.11
MR-3195	Jönköping	Sed., STP rec	Landsbro, Gröpplebäcken	ng/g DW	1.5	4.3	2.7	<2	4.1		1.4	<2	<0.7	0.34	<9	<47	<0.5	0.16
MR-3066	Jönköping	Sed., STP rec	Hultsfred, Hulingen	ng/g DW	2.9	8.9	5.7	10	<6	56	<12	<0.6	<1	9.0	<16	<9	<0.8	<0.2
MR-2971	Skåne	Sed., Coastal	Helsingborg (coast / harbour)	ng/g DW	12	5.8	0.31	<11	0.74	23	6.0	2.2		<2	<12	<1	<0.5	0.45

Table A 12. Concentration of methylphenols and long-chain alkylphenols in sediment.

Sample #	Prog.	Matrix	Site	Unit	2-Methyl-phenol	3-Methyl-phenol	4-Methyl-phenol	2,4-Dimethyl-phenol	3,5-Dimethyl-phenol	2,3-Dimethyl-phenol	3,4-Dimethyl-phenol	4-n-OP	4-t-OP	4-t-OP-EO1	4-t-OP-EO2	4-n-NP	4-NP	4-NP-EO1	4-NP-EO2	4-DP
MR-3043 (1)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<6	11	33	<65	8.5	10	3.4	<0.5	2.2	<3	1.2	<2	44	<140	<34	<6
MR-3043 (2)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<4	12	36	<84	4.7	10	3.0	<0.2	1.4	<2	<2	<4	96	210	<25	<12
MR-3043 (3)	nat	Sed., Backgr.	Ybbarpsjön 0-5 cm, upstream Perstorp	ng/g DW	<17	18	120	<140	12	31	6.8	<1	<2	<15	<3	<14	83	316	<44	<32
MR-3044 (1)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	<5	25	75	31	32	19	14	1.1	88	10	2.9	28	7700	870	340	<39
MR-3044 (2)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	<5	48	20	53	14	29	9.2	0.30	37	6.9	1.3	3.2	1400	220	50	<28
MR-3044 (3)	nat	Sed., ChemInd	Storarydsdammen 0-5 cm, downstream Perstorp	ng/g DW	<5	22	66	31	19	16	12	0.56	55	7.3	2.4	28	2500	450	150	<36
MR-2407	nat	Sed., ChemInd -coast	200m from point source, site A5	ng/g DW	<0.4	<0.6	29	<1	<0.5	<2	<0.9	0.029	0.17	<0.5	<0.2	<0.3	7.3	13	1.3	<0.8
MR-2409	nat	Sed., ChemInd -coast	1000 m from point source, site E1	ng/g DW	<0.7	<2	3300	<0.7	<1	<2	<1	<0.03	0.20	<0.7	0.14	<0.3	17	34	8.4	<2
MR-3049	nat	Sed., Backgr.	River, upstream anonymous point source	ng/g DW	<0.8	<0.9	3300	<4	<1	<3	<2	0.040	0.4	<2	0.17		12	<28	<6	<2
MR-3050	nat	Sed., ChemInd	River, downstream anonymous point source	ng/g DW	<3	9.0	6700	<5	<3	<8	2.0	<0.1	13	<8	2.1		1200	290	50	3.4
MR-3051	nat	Sed., ChemInd	River, downstream anonymous point source	ng/g DW	<2	8.4	5300	<4	<120	<170	1.6	<0.3	19	<13	3.3		1300	570	130	38
MR-3191	Värmland	Sed., ChemInd	Skoghall, Akzo Nobel, Anholms V	ng/g DW	500	890	11000	3500	590	270	250									
MR-3192	Värmland	Sed., ChemInd	Skoghallsådran, Akzo Nobel	ng/g DW	140	270	400	610	150	62	65									
MR-3193	Värmland	Sed., PaperInd	Skoghalls Bruk, Stora Enso	ng/g DW	15	3.6	730	<0.9	2.7	<2	<0.3									
MR-3194	Värmland	Sed., PaperInd	Grums, Billerud AB, Gruvöns bruk	ng/g DW	59	9.9	20000	3.5	2.8	1.7	3.8									
MR-2973	Värmland	Sed., PaperInd	Glafsåsjorden, fiberbank	ng/g DW	50	9.8	2700	3.3	2.1	2.3	0.090	0.48	42	<0.8	9.0	<19	560	300	240	<27
MR-3314	nat	Sed., Urban	Stockholm, Essingen 0-2 cm	ng/g DW	<0.7	<2	4200	<0.7	<1	<2	<1	<0.07	3.9	<3	0.71	<9	87	75	10	4.8
MR-3315	nat	Sed., Urban	Stockholm, Essingen 33-35 cm	ng/g DW	<0.9	10	460	<16	12	5.9	11	0.080	49	<2	0.99	<0.6	1100	220	26	5.7
MR-3316	nat	Sed., Urban	Stockholm, Riddarfjärden 0-2 cm	ng/g DW	<1	<12	3100	14	5.7	13	4.3	<0.1	7.5	<7	2.1	<6.7	120	150	28	<5
MR-3317	nat	Sed., Urban	Stockholm, Riddarfjärden 33-35 cm	ng/g DW	<0.7	9.5	1100	<19	16	7.3	11	<0.07	1.4	<1	<0.7	<0.4	<6	<35	<23	<3
MR-3318	nat	Sed., Urban	Stockholm, Årstaviken 0-2 cm	ng/g DW	<0.7	3.0	4100	2.1	1.5	0.9	1.6	<0.09	5.7	<5	1.9	<1	290	180	24	4.7
MR-3319	nat	Sed., Urban	Stockholm, Årstaviken 33-35 cm	ng/g DW	<0.8	6.4	110	<4	4.1	<4	5.5	<0.08	63	<6	5.3	<0.9	1900	500	88	9.1
MR-3059	Jönköping	Sed., Urban	Jönköping, Munksjön	ng/g DW	<6	<2	640	<23	9.9	<22	<6									
MR-3037	Jönköping	Sed., STP rec	Gislaved	ng/g DW																
MR-3195	Jönköping	Sed., STP rec	Landsbro, Gröpplebacken	ng/g DW	3.0	5.5	4000	<10	<2	<5	5.2									
MR-3066	Jönköping	Sed., STP rec	Hultsfred, Hulingen	ng/g DW																
MR-2971	Skåne	Sed., Coastal	Helsingborg (coast / harbour)	ng/g DW								0.48	43	<0.8	9.0	<19	560	300	240	<27

Table A 13. Concentration of tert butylphenols in soil.

Sample #	Prog.	Matrix	Site	Unit	2-t-Butylphenol	4-t-Butylphenol	2,6-Diisopropylphenol	6-t-Butyl-2,4-xyleneol	t-Butyl-4-hydroxyanisole	2,4-Di-tert-butylphenol	Isoeugenol	t-Butylhydroquinone	4-t-Butyltoluen	2,6-Di-tert-butylphenol	2,6-Diisobutylphenol	2,6-Di-tert-butyl-4-methylphenol	2,6-Di-tert-butyl-4-ethylphenol	2,4,6-Tri-tert-butylphenol
3353	nat	Soil	Trollhättan, Stallbacka	mg/kg DW	<0.0001	0.0014	<0.0002	<0.0004	<0.0002	0.0019	<0.0003	<0.0002	<0.0002	<0.0001	<0.002	<0.0001	<0.0001	<0.0001
3354	nat	Soil	Trollhättan, Stallbacka	mg/kg DW	<0.0001	0.0017	<0.0001	<0.0002	<0.0003	0.0010	<0.0002	<0.0002	<0.0002	<0.0001	<0.001	<0.0001	<0.0001	<0.0001
3355	nat	Soil	Trollhättan, Stallbacka	mg/kg DW	<0.0001	0.0006	<0.0001	<0.0004	<0.0002	0.0009	<0.0002	<0.0002	<0.0002	<0.0001	<0.001	<0.0001	<0.0001	<0.0001

Table A 14. Concentration of methylphenols and long-chain alkylphenols in soil.

Sample #	Prog.	Matrix	Site	Unit	2-Methylphenol	3-Methylphenol	4-Methylphenol	2,4-Dimethylphenol	3,5-Dimethylphenol	2,3-Dimethylphenol	3,4-Dimethylphenol	4-n-OP	4-t-OP	4-t-OP-EO1	4-t-OP-EO2	4-n-NP	4-NP	4-NP-EO1	4-NP-EO2	4-DP
3353	Nat	Soil	Trollhättan, Stallbacka	mg/kg DW	0.0024	0.0011	0.020	0.0052	0.0021	<0.001	0.0013	<0.002	0.0021	<0.001	<0.0003	<0.001	0.035	<0.014	<0.005	<0.002
3354	nat	Soil	Trollhättan, Stallbacka	mg/kg DW	0.0042	0.0022	0.020	0.0012	0.0005	<0.006	0.00036	<0.002	0.0011	<0.001	<0.0003	<0.0004	0.011	<0.025	<0.005	<0.002
3355	nat	Soil	Trollhättan, Stallbacka	mg/kg DW	0.0020	0.0004	0.021	0.0013	0.0006	<0.001	0.00049	<0.00004	0.0008	<0.001	<0.0003	<0.001	0.061	<0.025	<0.005	<0.002

Table A 15. Concentration of tert butylphenols in air.

Sample #	Matrix	Type	Site	Unit	2-t-Butyl-phenol	4-t-Butyl-phenol	2,6-Diisopropyl-phenol	6-t-Butyl-2,4-xyleneol	t-Butyl-4-hydroxy-anisole	2,4-Di-t-butyl-phenol	Iso-eugenol	t-Butylhydroquinone	4-t-Butyltoluen	2,6-Di-t-butyl-phenol	2,6-Di-isobutyl-phenol	2,6-Di-t-butyl-4-methylphenol	2,6-Di-t-butyl-4-ethylphenol	2,4,6-Tri-t-butylphenol
MR-3248	Air	Backgr.	Råö 031111-25	ng/m ³	<0.03	0.28	<0.03	<0.07	<0.05	<0.1	<0.1	<0.03	<0.2	<0.05	<0.27	<0.03	<0.01	<0.01
MR-3249	Air	Backgr.	Råö 031125-1209	ng/m ³	<0.06	<0.1	<0.07	<0.05	<0.02	<0.1	<0.16	<0.03	<0.2	0.070	<0.18	0.28	<0.01	<0.01
MR-3307	Air	Backgr.	Råö 031215-22	ng/m ³	<0.09	0.24	<0.03	<0.1	<0.05	<0.1	<0.16	<0.06	<0.2	<0.05	<0.45	0.14	<0.01	<0.01
MR-3320	Air	Backgr.	Pallas 031201-17	ng/m ³	<0.009	<0.1	<0.03	<0.04	<0.03	<0.1	<0.1	<0.03	<0.2	<0.05	<0.37	0.45	<0.01	<0.01
MR-3322	Air	Backgr.	Pallas 031217-31	ng/m ³	<0.07	<0.1	<0.05	<0.07	<0.04	<0.1	<0.1	<0.03	<0.2	<0.05	<0.38	0.18	<0.01	<0.01
MR-3067	Air	Ind	Malmö, Anonymous 031028-1104	ng/m ³	<0.01	0.16	<0.05	<0.06	<0.09	<0.1	<0.1	<0.06	<0.2	0.053	<0.37	<0.03	<0.01	<0.01
MR-3176	Air	Ind	Malmö, Anonymous 031111-1125	ng/m ³	<0.07	0.22	<0.06	<0.1	<0.06	<0.1	<0.1	<0.04	<0.2	0.10	<0.43	<0.03	<0.01	<0.01
MR-3240	Air	Ind	Malmö, Anonymous 031125-1212	ng/m ³	<0.04	0.11	<0.04	<0.1	<0.04	<0.1	<0.1	<0.05	<0.2	<0.05	<0.47	<0.03	<0.01	<0.01
MR-3117	Air	Ind	Perstorp 031029-1112	ng/m ³	<0.02	0.31	<0.03	<0.02	<0.04	<0.1	<0.1	<0.03	<0.2	0.33	<0.27	0.060	<0.01	<0.01
MR-3241	Air	Ind	Perstorp 031204-12	ng/m ³	<0.02	0.34	<0.03	<0.03	<0.05	<0.1	<0.1	<0.03	<0.2	0.10	<0.38	0.51	<0.01	<0.01
MR-3251	Air	Ind	Stenungsund 031125-1202	ng/m ³	<0.03	0.11	<0.03	<0.06	<0.03	<0.1	<0.1	<0.03	<0.2	<0.05	<0.15	0.35	<0.01	<0.01
MR-3252	Air	Ind	Stenungsund 031203-17	ng/m ³	<0.06	<0.1	<0.04	<0.09	<0.03	<0.1	<0.1	<0.03	<0.2	0.060	<0.39	1.0	<0.01	<0.01
MR-3254	Air	Ind	Trollhättan, Stallbacka 031201-16	ng/m ³	<0.007	<0.1	<0.03	<0.02	<0.02	<0.1	<0.1	<0.03	<0.2	<0.05	<0.1	0.092	<0.01	<0.01
MR-3275	Air	Ind	Trollhättan, Stallbacka 031216-30	ng/m ³	<0.01	<0.1	<0.03	<0.02	<0.02	<0.1	<0.1	<0.03	<0.2	<0.05	<0.14	0.084	<0.01	<0.01
MR-3262	Air	Urban	Malmö 031028-1112	ng/m ³	<0.3	0.15	<0.03	<0.04	<0.03	<0.1	<0.1	<0.03	<0.2	<0.05	<0.21	0.14	<0.01	<0.01
MR-3264	Air	Urban	Malmö 031113-1126	ng/m ³	<0.02	0.12	<0.03	<0.06	<0.02	<0.1	<0.1	<0.03	<0.2	<0.05	<0.15	0.077	<0.01	<0.01
MR-3266	Air	Urban	Malmö 031128-1212	ng/m ³	<0.01	<0.1	<0.03	<0.03	<0.04	<0.1	<0.1	<0.03	<0.2	0.093	<0.16	0.21	<0.01	<0.01
	Air	Urban	Stockholm 031020-29	ng/m ³	<0.02	<0.1	<0.03	<0.03	<0.02	<0.1	<0.1	0.080	<0.2	<0.05	<0.29	0.43	<0.01	<0.01
	Air	Urban	Stockholm 031029-1113	ng/m ³	<0.04	0.31	<0.07	<0.07	<0.03	<0.1	<0.1	0.048	<0.2	<0.05	<0.4	0.090	<0.01	<0.01

Table A 16. Concentration of methylphenols and long-chain alkylphenols in air.

Sample #	Matrix	Type	Site	Unit	2-Methyl-phenol	3-Methyl-phenol	4-Methyl-phenol	2,4-Di-methyl-phenol	3,5-Di-methyl-phenol	2,3-Di-methyl-phenol	3,4-Di-methyl-phenol	4-n-OP	4-t-OP	4-t-OP-EO1	4-t-OP-EO2	4-n-NP	4-NP	4-NP-EO1	4-NP-EO2	4-DP
MR-3248	Air	Backgr.	Råö 031111-25	ng/m ³	<1	1.5	2.5	1.1			0.37	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3249	Air	Backgr.	Råö 031125-1209	ng/m ³	3.3	<1	1.6	0.78			0.62	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3307	Air	Backgr.	Råö 031215-22	ng/m ³	<1	<1	1.5	0.43			<0.3	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3320	Air	Backgr.	Pallas 031201-17	ng/m ³	<1	<1	0.45	0.26			<0.3	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3322	Air	Backgr.	Pallas 031217-31	ng/m ³	<1	<1	0.25	0.23			<0.3	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3067	Air	Ind	Malmö, Anonymous 031028-1104	ng/m ³	<1	3.3	4.8	3.0			1.4	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3176	Air	Ind	Malmö, Anonymous 031111-1125	ng/m ³	1.2	5.2	3.9	4.3			2.3	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3240	Air	Ind	Malmö Anonymous 031125-1212	ng/m ³	2.0	1.9	2.5	2.8			1.7	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3117	Air	Ind	Perstorp 031029-1112	ng/m ³	<1	1.3	3.3	1.0			0.40	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3241	Air	Ind	Perstorp 031204-12	ng/m ³	1.5	3.4	2.1	1.8			1.1	<0.3	<0.3	<0.1	<0.1	<0.05	0.29	<0.3	<0.3	<0.3
MR-3251	Air	Ind	Stenungsund 031125-1202	ng/m ³	<1	2.9	2.0	2.0			1.0	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3252	Air	Ind	Stenungsund 031203-17	ng/m ³	<1	4.1	2.1	1.6			1.3	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3254	Air	Ind	Trollhättan, Stallbacka 031201-16	ng/m ³	9.0	5.3	7.5	2.8			2.1	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3275	Air	Ind	Trollhättan, Stallbacka 031216-30	ng/m ³	12	9.4	7.0	3.7			1.7	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3262	Air	Urban	Malmö 031028-1112	ng/m ³	3.4	2.8	2.4	1.2			0.68	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
MR-3264	Air	Urban	Malmö 031113-1126	ng/m ³	3.9	4.1	3.7	1.8			1.1	<0.3	<0.3	<0.1	<0.1	<0.05	2.85	<0.3	<0.3	<0.3
MR-3266	Air	Urban	Malmö 031128-1212	ng/m ³	<1	3.3	5.2	3.7			1.6	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
	Air	Urban	Stockholm 031020-29	ng/m ³	1.4	2.4	1.5	3.0			1.8	<0.3	<0.3	<0.1	<0.1	<0.05	<0.3	<0.3	<0.3	<0.3
	Air	Urban	Stockholm 031029-1113	ng/m ³	2.6	3.2	3.3	3.7			2.2	<0.3	<0.3	<0.1	<0.2	<0.05	<0.3	<0.3	<0.3	<0.3

Table A 17. Concentration of tert butylphenols in fish.

Sample #	Prog.	Site	Unit	% lipid of fw	2-tert- Butyl- phenol	4-tert- Butyl- phenol	2,6-Diiso- propyl- phenol	6-tert-Butyl- 2,4-xyleneol	tert-Butyl-4- hydroxy- anisole	2,4-Di-tert- butyl-phenol	Iso- eugenol	tert-Butyl- hydro- quinone	4-tert- Butyl- toluen	2,6-Di-tert- butyl-phenol	2,6-Di-iso- butyl-phenol	2,6-Di-tert- butyl-4-methyl- phenol	2,6-Di-tert- butyl-4-ethyl- phenol	2,4,6-Tri-tert- butyl-phenol
MR-2955	Skåne	Finjasjön (Hässleholm), perch	ng/g fw	0.89	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2956	Skåne	Ivösjön (Bromölla, Kristianstad), perch	ng/g fw	0.81	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2957	Skåne	Ringsjön (Höör, Hörby), perch	ng/g fw	0.92	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2958	Skåne	Storarydsdammen (Perstorp, Klippan), perch	ng/g fw	0.77	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2959	Skåne	Stora damm/Fåglasjön (Perstorp, Hässleholm), perch	ng/g fw	0.78	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2960	Skåne	Fjällfotasjön (Svedala), perch	ng/g fw	0.79	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2961	Skåne	Västersjön/Rössjön (Ängelholm), perch	ng/g fw	0.81	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2962	Skåne	Krageholmsjön (Ystad), perch	ng/g fw	0.80	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-2972	Skåne	Helsingborg R3, flounder	ng/g fw	0.79	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<4	<0.5	<0.1	<0.1	<0.1
MR-3038	Skåne	Spillepeng, (Helsingborg), perch	ng/g fw	0.79	<3	<3	<3	<3	<3	<2	<3	<3	<0.2	<6	<0.8	<0.2	<0.2	<0.2
MR-3350	nat	Fladen P2002/1482-86, herring	ng/g fw	3.5	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<0.1	<4	<0.5	<0.1	<0.1
MR-3351	nat	Fladen P2002/1487-91, herring	ng/g fw	3.9	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<0.1	<4	<0.5	<0.1	<0.1
MR-3352	nat	Fladen P2002/1492-96, herring	ng/g fw	4.0	<2	<2	<2	<2	<2	<2	<2	<2	<0.1	<0.1	<4	<0.5	<0.1	<0.1

Table A 18. Concentration of methylphenols and long-chain alkylphenols in fish.

Sample #	Prog.	Site	Unit	% lipid of fw	2-Methyl- phenol	3-Methyl- phenol	4-Methyl- phenol	2,4-Di- methyl- phenol	3,5-Di- methyl- phenol	2,3-Di- methyl- phenol	3,4-Di- methyl- phenol	4-n-OP	4-t-OP	4-t-OP- EO1	4-t-OP- EO2	4-n-NP	4-NP (i.m.)	4-NP-EO1 (i.m.)	4-NP-EO2 (i.m.)	4-DP (i.m.)
MR-2955	Skåne	Finjasjön (Hässleholm), perch	ng/g fw	0.89								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2956	Skåne	Ivösjön (Bromölla, Kristianstad), perch	ng/g fw	0.81								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2957	Skåne	Ringsjön (Höör, Hörby), perch	ng/g fw	0.92								<2	<0.3	<2	<2	<2	15	<20	<10	<10
MR-2958	Skåne	Storarydsdammen (Perstorp, Klippan), perch	ng/g fw	0.77								<2	1,3	<2	<2	<3	<10	<20	<10	<10
MR-2959	Skåne	Stora damm/Fåglasjön (Perstorp, Hässleholm), perch	ng/g fw	0.78								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2960	Skåne	Fjällfotasjön (Svedala), perch	ng/g fw	0.79								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2961	Skåne	Västersjön/Rössjön (Ångelholm), perch	ng/g fw	0.81								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2962	Skåne	Krageholmssjön (Ystad), perch	ng/g fw	0.80								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-2972	Skåne	Helsingborg R3, flounder	ng/g fw	0.79								<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-3038	Skåne	Spillepeng (Helsingborg), perch	ng/g fw	0.79								<3	<0.5	<3	<3	<3	<6	<14	<8	<8
MR-3350	nat	Fladen P2002/1482-86, herring	ng/g fw	3.5	<5	<5	<5	<5	<5	<5	<5	<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-3351	nat	Fladen P2002/1487-91, herring	ng/g fw	3.9	<5	<5	<5	<5	<5	<5	<5	<2	<0.3	<2	<2	<2	<10	<20	<10	<10
MR-3352	nat	Fladen P2002/1492-96, herring	ng/g fw	4.0	<5	<5	<5	<5	<5	<5	<5	<2	<0.5	<2	<2	<2	<10	<20	<10	<10

Table A 19. Physical- Chemical properties used. All phys-chem data were taken from databases, and except for obvious erratic data, the authors did not critically review these data.

CAS nr	Name	MW (g/mol)	Wsol (mg/L)	Vp (Pa)	Log Kow	MP (°C)	Pka	Half-life (h)				Reference
								Air	Water	Soil	Sediment	
Tert butylphenols												
88-18-6	2-tert-butylphenol	150	700	12 ^a	3.3	-6.8	10	6.3	900	900	3600	SRC, 2003
98-54-4	4-tert-butylphenol	150	580	5.1	3.3	98	10	6.3	900	900	3600	SRC, 2003
2078-54-8	2,6-diisopropylphenol	178	120 ^b	0.41 ^b	3.8	18	11	4.9	900	900	3600	SRC, 2003
1879-09-0	6-tert-butyl-2,4-xylene	178	27 ^b	6.0 ^a	4.5 ^b	22	12	12	900	900	3600	SRC, 2003
8003-24-5. 25013-16-5	tert-butyl-4-hydroxyanisole	361	210 ^b	0.33 ^b	3.5 ^b	51		7.1	900	900	3600	SRC, 2003
96-76-4	2,4-di-tert-butylphenol	206	35	0.63 ^a	5.2	56	12	5.2	900	900	3600	SRC, 2003
97-54-1	Isoeugenol	164	360 ^b	1.6 ^a	3.0	-10	10	1.7	360	360	1440	SRC, 2003
1948-33-0	tert-butylhydroquinone	166	750 ^b	0.029 ^b	2.9 ^b	83 ^b		5.0	900	900	3600	EPIWIN (Meylan, 1999)
98-51-1	4-tert-butyltoluene	148	5.5 ^b	89 ^b	5.2	-52		18	900	900	3600	SRC, 2003
128-39-2	2,6-di-tert-butylphenol	206	2.5	0.97 ^b	4.9	39	12	5.2	900	900	3600	SRC, 2003
52348-51-3	2,6-diisobutylphenol	206	3.7 ^b	0.041 ^b	5.4 ^b	76 ^b		4.5	900	900	3600	EPIWIN (Meylan, 1999)
128-37-0	2,6-di-tert-butyl-4-methylphenol	220	0.6	0.69 ^a	5.1	71	12	14	900	900	3600	SRC, 2003
4130-42-1	2,6-di-tert-butyl-4-ethylphenol	234	2.1 ^b	0.29 ^b	5.5 ^b	44		14	1440	1440	5760	EPIWIN (Meylan, 1999)
732-26-3	2,4,6-tri-tert-butylphenol	262	35	0.088 ^a	6.1	131	12	16	1440	1440	5760	SRC, 2003
Methylphenols												
95-48-7	2-methylphenol	108	2.6×10 ⁴	40 ^a	2.0	30	10	6.1	360	360	1440	SRC, 2003
108-39-4	3-methylphenol	108	2.3×10 ⁴	15	2.0	12	10	4.0	360	360	1440	SRC, 2003
106-44-5	4-methylphenol	108	2.2×10 ⁴	15	1.9	36	10	5.4	360	360	1440	SRC, 2003
105-67-9	2,4-dimethylphenol	122	7.9×10 ⁴	14	2.3	25	11	3.6	360	360	1440	SRC, 2003
108-68-9	3,5-dimethylphenol	122	4.9×10 ³	5.4 ^a	2.4	64	10	2.3	360	360	1440	SRC, 2003
526-75-0	2,3-dimethylphenol	122	4.6×10 ³	12 ^a	2.5	73	11	3.2	360	360	1440	SRC, 2003
95-65-8	3,4-dimethylphenol	122	4.8×10 ³	4.7 ^a	2.2	61	12	3.2	360	360	1440	SRC, 2003
Alkylphenols												
1806-26-4 27193-28-8	4-octylphenol	206	3.1 ^b	0.013 ^b	5.5 ^b	83 ^b		5.1	360	360	1440	EPIWIN (Meylan, 1999)

Table A 19. Cont.

CAS nr	Name	MW (g/mol)	Wsol (mg/L)	Vp (Pa)	Log Kow	MP (°C)	Pka	Half-life (h)			Reference
140-66-9	4-tert-octylphenol	206	5.0 ^b	0.064 ^a	5.3 ^b	85	6.1	900	900	3600	SRC, 2003
1322-97-0	4-tert-octylphenol-mono-ethoxylate	250	4.5 ^b	1.5×10 ⁻⁴ . ^b	5.0 ^b	91 ^b	4.8	360	360	1440	EPIWIN (Meylan, 1999)
25154-52-3	n-nonylphenol	220	6.4	3.1×10 ⁻³	6.0	42	5.0	360	360	1440	SRC, 2003
104-40-5	4-nonylphenol	220	7.0	0.11	5.8	42	5.0	360	360	1440	SRC, 2003
84852-15-3	4-nonylphenol, branched (i.m.)	220	6.0	0.013	5.9 ^b	90	5.0	900	900	3600	SRC, 2003; ECB, 2002
9016-45-9	4-nonylphenol-ethoxylate	264	1.4 ^b	5.5×10 ⁻⁵ . ^b	5.5 ^b	100 ^b	4.7	360	360	1440	EPIWIN (Meylan, 1999)
27193-86-8	4-dodecylphenol	262	0.032 ^b	3.1×10 ⁻⁴ . ^b	6.6 ^b	117 ^b	2.6	360	360	1440	SRC, 2003; EPIWIN (Meylan, 1999)

^aExtrapolated value

^bEstimated value

Table A 20. Results from triplicate sampling of sediments upstream and downstream of a chemical industry #1. Levels in ng/g dw. OP:octylphenol; NP:nonylphenol. C.V. = relative standard deviation.

	Upstream			Downstream			C.V. upstr.	C.V. downst.	p (t-test)
	#1	#2	#3	#1	#2	#3			
2-t-Butylphenol	<1	<1.3	<1.9	0.77	1.4	1.3		29.3%	
4-t-Butylphenol	<0.99	<1.3	<3.1	18	14.5	28		35.6%	
2,6-Diisopropyl-phenol	<0.84	<0.54	<1.6	0.6	0.54	0.3		33.1%	
6-t-Butyl-2,4-xyleneol	<2.1	<1.4	<4.1	3.3	3	1.3		42.6%	
t-Butyl-4-hydroxyanisole	<1.5	<1.9	<5.8	0.78	2.9	0.73		84.3%	
2,4-Di-t-Butylphenol	<2.4	<1.3	<3.2	5.5	3.4	6.3		29.5%	
Isoeugenol	<2.1	<2.7	<13	7.6	14	16		35.5%	
t-Butylhydroquinone	<2.0	<1.9	3.5	2.7	2.6	2.5		3.5%	
4-t-Butyltoluene	<2.4	<1.24	<1.6	<0.41	<0.5	<0.53			
2,6-Di-t-Butylphenol	<1.6	<0.85	<1.11	<0.03	<0.34	1.2			
2,6-Diiso-Butylphenol	<19	<12	<36	<12	<12	<11			
2,6-Di-t-butyl-4-methylphenol	<1.8	<0.93	<1.2	1.5	<0.9	2.1		25.4%	
2,6-Di-t-butyl-4-ethylphenol	<1.6	<0.82	<1.07	<0.27	<0.5	<0.35			
2,4,6-Tri-t-Butylphenol	<1.1	<0.58	<0.76	0.15	0.07	0.23		53.3%	
2-Methylphenol	<6.2	<4.1	<17	<4.5	<5.1	<4.6			
3-Methylphenol	11	12	18	25	48	22	27.7%	44.6%	0.099
4-Methylphenol	33	36	117	75	20	66	76.9%	55.0%	0.81
2,4-Dimethylphenol	<65	<84	<138	31	53	31		33.1%	
3,5-Dimethylphenol	8.5	4.7	12	32	14	19	43.5%	42.9%	0.083
2,3-Dimethylphenol	10	10	31	19	29	16	71.3%	31.9%	0.62
3,4-Dimethylphenol	3.4	3	6.8	14	9.2	12	47.5%	20.5%	0.016
4-n-OP	<0.46	<0.24	<1.1	1.1	0.3	0.56		62.5%	
4-t-OP	2.2	1.4	<1.7	88	37	55	31.4%	43.1%	0.06
4-t-OP-EO1	<2.7	<1.7	<15.2	10	6.9	7.3		20.9%	
4-t-OP-EO2	1.2	<1.9	<3.3	2.9	1.3	2.4		37.2%	
4-n-NP	<1.9	<3.6	<14.3	27.7	3.2	27.7		72.4%	
4-NP (i.m.)	44	96	83	7735	1401	2470	36.4%	87.6%	0.1
4-NP-EO1	<137	210	316	865	221	452	28.5%	63.6%	0.385
4-NP-EO2	<34	<25	<44	336	50	149		81.4%	
4-Dodecylphenol	<6	<12	<31.6	<38.7	<27.5	<36.4			



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