SUSPECT SCREENING IN NORDIC COUNTRIES

POINT SOURCES IN CITY AREAS

Suspect screening in Nordic countries

Point sources in city areas

*Martin Schlabach, Peter Haglund, Malcolm Reid, Pawel Rostkowski,
Cathrin Veenaas, Kine Bæk and Bert van Bavel*

Suspect screening in Nordic countries

Point sources in city areas

Martin Schlachach, Peter Haglund, Malcolm Reid, Pawel Rostkowski, Cathrin Veenaas, Kine Bæk and Bert van Bavel

ISBN 978-92-893-5199-7 (PRINT)

ISBN 978-92-893-5200-0 (PDF)

ISBN 978-92-893-5201-7 (EPUB)

<http://dx.doi.org/10.6027/TN2017-561>

TemaNord 2017:561

ISSN 0908-6692

Standard: PDF/UA-1

ISO 14289-1

© Nordic Council of Ministers 2017

Cover photo: unsplash.com

Print: Rosendahls

Printed in Denmark

Disclaimer

This publication was funded by the Nordic Council of Ministers. However, the content does not necessarily reflect the Nordic Council of Ministers' views, opinions, attitudes or recommendations.

Rights and permissions

This work is made available under the Creative Commons Attribution 4.0 International license (CC BY 4.0) <https://creativecommons.org/licenses/by/4.0>.

Translations: If you translate this work, please include the following disclaimer: *This translation was not produced by the Nordic Council of Ministers and should not be construed as official. The Nordic Council of Ministers cannot be held responsible for the translation or any errors in it.*

Adaptations: If you adapt this work, please include the following disclaimer along with the attribution: *This is an adaptation of an original work by the Nordic Council of Ministers. Responsibility for the views and opinions expressed in the adaptation rests solely with its author(s). The views and opinions in this adaptation have not been approved by the Nordic Council of Ministers.*

Third-party content: The Nordic Council of Ministers does not necessarily own every single part of this work. The Nordic Council of Ministers cannot, therefore, guarantee that the reuse of third-party content does not infringe the copyright of the third party. If you wish to reuse any third-party content, you bear the risks associated with any such rights violations. You are responsible for determining whether there is a need to obtain permission for the use of third-party content, and if so, for obtaining the relevant permission from the copyright holder. Examples of third-party content may include, but are not limited to, tables, figures or images.

Photo rights (further permission required for reuse)

Any queries regarding rights and licences should be addressed to:

Nordic Council of Ministers/Publication Unit
Ved Stranden 18
DK-1061 Copenhagen K
Denmark
Phone +45 3396 0200
pub@norden.org

Nordic co-operation

Nordic co-operation is one of the world's most extensive forms of regional collaboration, involving Denmark, Finland, Iceland, Norway, Sweden, and the Faroe Islands, Greenland and Åland.

Nordic co-operation has firm traditions in politics, economics and culture and plays an important role in European and international forums. The Nordic community strives for a strong Nordic Region in a strong Europe.

Nordic co-operation promotes regional interests and values in a global world. The values shared by the Nordic countries help make the region one of the most innovative and competitive in the world.

The Nordic Council of Ministers

Nordens Hus
Ved Stranden 18
DK-1061 Copenhagen K, Denmark
Tel.: +45 3396 0200 www.norden.org

Download Nordic publications at www.norden.org/nordpub

Contents

Preface	7
Summary	9
1. Introduction	13
2. Methodology	15
2.1 Sampling	15
2.2 Chemical Laboratory Work	17
2.3 Compound identification (Post-acquisition Data Treatment)	21
3. Results and Discussion	27
3.1 Results from target and suspect screening	27
3.2 Comparison of effluent water concentrations	32
4. Conclusions	35
5. Acknowledgements	37
5.1 Denmark	37
5.2 Faroe Islands	37
5.3 Finland	37
5.4 Greenland	37
5.5 Iceland	37
5.6 Norway	38
5.7 Sweden	38
References	39
Sammendrag	41
Appendix	45

Preface

The aim of the Nordic environmental screening is to obtain a snapshot of the occurrence of potentially hazardous substances, both in regions most likely to be polluted as well as in some pristine environments. The focus is on less known, anthropogenic substances and their derivatives, which either are used in high volumes or are likely to be persistent and hazardous to humans and other organisms.

The project steering group has initiated a non-targeted screening of possible environmental pollutant in selected samples from point-sources in cities in 2015. The method “non-target screening”, as defined in the invitation for tender, is a technique that can identify environmental pollutants without a preceding selection of the compounds of interest. The Nordic screening group wants to use the non-target screening method to discover emerging pollutants in the Nordic environment-impact both from small cities as in Greenland and larger cities as in Sweden. The result is expected to be used for later targeted studies and in international chemical regulation processes like REACH and the Stockholm POP convention.

The following Nordic countries and self-governing areas are included in the project: Finland, Sweden, Norway, Denmark, Faroe Islands, Iceland and Greenland.

The matrices selected for the analyses are:

- Effluent water from waste water lines or treatment plants.
- Sediments from receiving waters (whether marine or freshwater as decided by each country).
- Fish from receiving waters (marine or freshwater as decided by each country).

The Nordic screening project is run by a steering group with representatives from Danish Centre for Environment and Energy, Aarhus University, Denmark, Finnish Environment Institute, Environment Agency of Iceland, the Environment Agency of the Faroe Islands, the Norwegian Environment Agency, Greenland Institute of Natural Resources and the Swedish Environmental Protection Agency. The project is financed and supported by the Nordic Council of Ministers through the Nordic Chemicals Group and the Marin Group (HAV) as well as the participating institutions.

The chemical analyses have been carried out jointly by NILU-Norwegian Institute for Air Research, Norwegian Institute for Water Research (NIVA), and Umeå University Department of Chemistry. The respective participating Nordic countries organised sample selection, collection and transport of samples based on a sample protocol and manuals provided by the analytical laboratories.

Summary

On behalf of the Nordic Council of Ministers through the Nordic Chemicals Group, and the Marin Group (HAV) NILU-Norwegian Institute for Air Research, Norwegian Institute for Water Research (NIVA), and Umeå University Department of Chemistry jointly performed a suspect screening study in effluent, sediment, and fish samples from all seven Nordic countries.

This study was originally planned as non-target screening. However, as the non-target screening approach is under rapid development and different data treatment approaches are tested, it became necessary to distinguish clearly between the different approaches and “suspect screening” is coming up as a new term or concept. The original concept non-target screening is now replaced by two concepts, namely suspect screening and non-target screening in a more strict definition, and only the time efficient suspect screening approach was applied here.

The respective participating Nordic countries organised sample selection, collection and transport of samples based on a sample protocol and manuals provided by the analytical laboratories. Each country sampled one effluent water sample (single/grab sample) from a major sewage treatment plant. In addition, it was also sampled one sediment sample (single/grab sample) and one fish sample (pooled sample) each. These environmental samples were taken close to the effluent emission samples except the Danish samples of sediment and fish. For this study a generic extraction and clean-up of samples was carried out at NIVA, Oslo, Norway. To cover a broadest possible range of compound groups two different extraction and clean-up methods were applied. The first method is optimized for non-polar and very lipophilic compounds like PCBs, PAHs and other classical POPs, and the second is optimized for polar compounds like pharmaceuticals, modern pesticides and biocides, PFAS, and bisphenols. Prior to extraction, samples were spiked with a number of isotopically labelled internal standards. The final extracts were sent to the different laboratories of the project group.

To cover a broad spectra of different compounds both GC- and LC-MS was applied (1. GCxGC-HRMS, 2. GC-ECNI-HRMS, 3. LC-QToFMS ESI+, and 4. LC-QToFMS ESI-). Raw data from all analyses in the project (in the format native to the instrument it was obtained) is being stored at NILU datacenter at secured, fully backed up FTP server. In a first step of raw data treatment important information of the mass spectrometric peaks as the mass centroid positions of the peaks, their areas under curve and full-width-at-half-maxima are extracted from the raw MS data and stored for further treatment. The next and most efficient step of post acquisition data treatment is normally filtration of the list of mass spectra of interest against libraries of suspect compounds. These libraries are either home-made, from commercial supplies or from the NORMAN network and are the most critical part of the suspect screening approach.

Suspect screening leads directly to tentative candidates with evidence for possible structure(s), but insufficient information for the exact structure.

It was possible to identify and partly (semi)quantify: Per- and polyfluorinated compounds (PFC), chlorinated and brominated compounds, different flame retardants, bisphenols, polycyclic aromatic compounds (PAC), industrial additives like UV-stabilizers, antioxidants, and plasticizers, and pharmaceuticals and personal care products (PPCP). When identified by GC the concentration was estimated in a semi-quantitative way. However, today it is not yet possible to estimate concentrations, when using LC-MS technology.

There are identified several compounds, which might be interesting and relevant for further in depth studies:

- Emerging PFAS compounds like 4:2 FTMAC (1799-84-4), 4:3 Acid (80705-13-1), C6/C6-PFPIA (40143-77-9), FOSA (754-91-6), 4:2 FTAL (135984-67-7), and 4:2 FTOH (2043-47-2) were identified in sediments.

In the sediment sample from Sweden several chlorinated aromatic compounds were found: 3,4,5-trichlorobenzenamine (634-91-3), 1-chloro-3-isocyanatobenzene (2909-38-8), and dichloro and trichloroaniline (CAS 608-27-5 and 634-91-3). Several substituted aniline derivatives are used in the production of dyes and herbicides and these findings may be related to emissions from industrial processes.

Several new bisphenols (S, E, and AF) were identified, and most concerning even in fish samples.

Numerous industrial additives were found in sediment, water and fish samples. These were for instance phenols, UV-stabilizers, antioxidants, and plasticizers of phthalate-type. Also a benzothiazole compound (2-methylthiobenzothiazole, MTBT, CAS: 615-22-5) was frequently found in all sample types and in high concentrations. 2-Methylthiobenzothiazole is a degradation product of mercaptobenzothiazol (MBT, CAS: 149-30-4), which is used in vulcanization of rubber. MTBT has earlier been detected in other screening studies in water and other abiotic samples, however, to our best knowledge not yet in marine biota.

A huge number of pharmaceuticals were identified in effluent samples. Many of the identified pharmaceuticals are not only found in effluents from sewage treatment plants (STPs) with basic or no treatment, but also in STPs with advanced treatment technologies. The effluent water samples are similar enough to allow a comparison of contaminant levels. The concentrations in effluents from STPs with advanced sewage treatment (SE, DK, FI, NO) vs. STPs with basic or no treatment (FO, IS, GL) is likely to reflect the relative persistency of relatively water soluble contaminants. The terpenoids coumarin, carvone, menthol and tetrahydralinalol and the alkaloid caffeine are, for instance, much less abundant in effluent from STPs with advanced treatment. It is plausible that those are degraded in the activated sludge process. However, for a number of contaminants like m-Cresol, 2-(Methylthio)pyridine, 2-(Methylthio)benzothiazole, 9-methylacridine, 3,3-Diphenylacrylonitrile, 3,3-Diphenylpropionitrile, N-butyl-benzenesulfonamide, and Diclofenac the levels were

highest in effluent from one of the STPs in SE, DK or FI, likely because of higher load from industry, traffic and other urban sources.

With an initial suspect data treatment using different mass spectral data bases it was possible to detect and identify a surprisingly long list of compounds of possible emerging concern with a level of confidence of three or better. When evaluating the total outcome of this study, it is important to keep the following limitations in mind: In order to get a wide overview over all anthropogenic compounds in environmental samples, a general sample preparation method has to be chosen. Many compounds, which easily could be detected by a dedicated target method, will be masked or lost either by (1) interfering matrix, (2) instrumental overload/saturation, and/or (3) possible loss of compounds. Furthermore, the applied GC/LC methods are often not optimal for each single analyte. For the time being, suspect/non-target screening cannot replace dedicated target methods in sensitivity and specificity, but it has proven to be an important tool for identification of compounds of emerging concern.

1. Introduction

Today, the monitoring of the environmental level of organic potentially hazardous compounds is mainly based on the use of mass spectrometers. The applied techniques can be classified either as target or non-target methods, that means either selecting the compounds of interest before starting the analysis or at a later stage. Traditional environmental monitoring of organic pollutants as PCB or chlorinated pesticides is targeting specific compounds, and is therefore named target analysis. In contrast, non-target analysis or non-target screening is defined as an analytical technique that can identify environmental pollutants without selection of the compounds of interest before starting the chemical analysis. This understanding of non-target screening is also at the base of the invitation to tender of this project.

Target analysis starts with optimizing the sample extraction and clean-up, and instrumental method to the beforehand selected analytes. This means that the complete analytical workflow including extraction, clean-up, and detection are optimized to provide a specific and accurate measurement (Thomas *et al.*, 2015). Most of the target analytical methods are quantitative, a feature that is often facilitated by using isotopically labeled internal standards that are analogues of the target analytes.

Non-target analysis has always existed in parallel to target analysis. However, the earlier instruments were not appropriate for applying non target analysis on a routine base and sufficient sensitivity. Over the past years, mass spectrometers used for environmental analysis have developed considerably. The major revolution in instrument technology is a new generation of accurate mass or high-resolution mass spectrometers (HRMS), which now allow the acquisition of a full spectrum of compounds with the same sensitivity which earlier were possible with only some very few selected compounds. These new instruments widens the applicability of non-target screening also onto environmental samples.

Both suspect and non-target screening are using HRMS and are complementary to targeted analysis, as shown and explained in (Figure 3) and chapter 2.3.

Similarly to target analysis, suspect screening uses some form of prior knowledge to search for the presence of a substance in a sample, however, without the use of a reference standards. Instead the exact mass, isotope pattern and chromatographic retention time is used. There are a large number of different databases and libraries available that can be used to perform the suspect screening process, such as those sold by instrument producers and those in the public domain, such as STOFF-IDENT (<https://www.lfu.bayern.de/stoffident/#!/home>), MassBank (<https://massbank.eu/MassBank/>) or ChemSpider (<http://www.chemspider.com/>). A prioritized list of compounds, which one would expect to find in the environment, is essentially the most effective suspect list for environmental screening. This list must be supported with the necessary information to identify the compounds in accurate mass

full-scan chromatograms. The Norman Network is working towards creating a common suspect screening list through exchanging information and this will be freely available (<http://www.norman-network.com/?q=node/236>).

Non-target screening in the new and stricter understanding, involves the identification of peaks in the chromatogram that are unknown and about which no prior information is known. This typically involves the selection of peaks (that have not been identified by suspect or target analysis) based upon their intensity (size) and the absence in control/blank samples. Each peak is then identified based on the accurate mass measurement that is used to generate the most plausible molecular formula, a process that is often complimented by the use of MS/MS fragment data. Such data can then be compared with libraries and/or various in silico fragmentation platforms to identify candidates.

Any screening without reference standards carries a level of uncertainty. Schymanski *et al.*, have proposed a matrix, which connects the different identification approaches versus the confidence in identification levels. A slightly adapted version of this matrix is shown in Figure 3, which in contrast to the matrix of Schymanski, also show the traditional target analysis approach. A high quality target method is normally based on the use of calibration or reference standards and internal standards and will end up at level 0, which is not included in the Schymanski matrix. For a compound at confidence level 0 the chemical structure is confirmed, and in addition also the concentration is known. At level 1 (the best level in the Schymanski matrix) only the structure is determined by comparison to an authentic reference standard and confirmation with MS, MS/MS and retention time matching. Level 2 is described as the possible structure provided by a match with library spectra and/or other diagnostic evidence, and level 3 as a tentative candidate based upon evidence for a possible structure, but where there is insufficient information for identification to exact structure. Level 4 describes the unequivocal molecular formula and level 5 the exact mass of the molecular ion. For the purpose of this report, only compounds identified with a confidence of level 0 to 3 are reported.

2. Methodology

2.1 Sampling

Co-ordination of sampling was supervised by NIVA, whereas the practical work was done or coordinated by the seven participating Nordic institutions in accordance with the Sampling Protocol as shown in the Appendix. This sampling protocol was prepared by the contracted institutes and adopted by the Steering Group. Each country sampled one effluent water sample (single/grab sample) from a major sewage treatment plant. In addition, it was also sampled one sediment sample (single/grab sample), and one fish sample (pooled sample) each (Table 1). These environmental samples were taken close to the effluent emission samples except the Danish samples of sediment and fish (see also Table 2).

Figure 1: Sampling stations

Note: Sampling of effluent water, sediment, and fish samples was done by the national collaborators.

Source: Google Maps.

Table 1: Sampling stations

Matrix	Sample ident.	Location	Site	Latitude	Longitude	Number of subsamples
Effluent	FO-1-Eff	Torshavn	UA 11 (Sersjantvikin)	62.00783	-6.76132	1
Sediment	FO-1-Sed	Torshavn	UA 17 (Alakeri)	62.00225	-6.77287	1
Fish Coalfish	FO-1-Fis	Torshavn	UA11 og UA17	62.00225	-6.77287	20
Effluent	DK-1-Eff	Aarhus	Marselisborg WWTP	56.23400	10.34995	1
Sediment	DK-1-Sed	Roskilde	Ros 60	55.70783	12.06667	1
Fish Eel pout	DK-1-Fis	Roskilde	Risø	55.68833	12.07500	28
Effluent	FI-1-Eff	Helsinki	Viikinmäki	60.22670	24.99645	1
Sediment	FI-1-Sed	Helsinki	Vanhankaupunginselkä	60.20083	24.99463	1
Fish Perch	FI-1-Fis	Helsinki	Vanhankaupunginselkä	60.20083	24.99463	23
Effluent	SE-1-Eff	Stockholm	Henriksdal WWTP	59.30975	18.10763	1
Sediment	SE-1-Sed	Stockholm	Henriksdal WWTP	59.32025	18.13525	1
Fish Perch	SE-1-Fis	Stockholm	Henriksdal WWTP	59.32025	18.13525	8
Effluent	GL-1-Eff	Nuuk	Kakillarnat	64.19687	-51.70252	1
Sediment	GL-1-Sed	Nuuk	Kakillarnat	64.19692	-51.70575	1
Fish Cod	GL-1-Fis	Nuuk Fiord	Kakillarnat	64.19748	-51.70528	5
Effluent	IS-1-Eff	Reykjavik	Klettagardar WWT	64.15553	-21.87275	1
Sediment	IS-1-Sed	Reykjavik	Inner Faxafloi bay	64.19228	-21.92260	1
Fish Cod	IS-1-Fis	Reykjavik	Inner Faxafloi bay	64.19228	-21.92260	5
Effluent	NO-1-Eff	Oslo	VEAS	59.79319	10.49958	1
Sediment	NO-1-Sed	Oslo	Oslofjord	59.79018	10.51922	1
Fish Cod	NO-1-Fis	Oslo	Oslofjord	59.79018	10.51922	5

Note: Station coordinates are given as WGS84 geographic coordinates in decimal degrees.
The biota sample of each country is one pooled samples, where the number of subsamples are listed in the table.

Effluent from Faroe Islands were sampled at the Sersjantvikin WWTP, Torshavn. The Sersjantvikin WWTP, Torshavn, receives domestic wastewater only and from approx. 1,000 pe. This WWTP may be described as consisting of a primary purification step (Kaj, Wallberg, & Brorström-Lundén, 2014).

Effluent from Denmark were sampled at the Marselisborg WWTP, Aarhus. The Marselisborg WWTP, Aarhus, receives domestic, industrial and hospital wastewater from approx. 200,000 pe. This WWTP may be described as state-of-the art WWTP.

Effluent from Finland were sampled at the Viikinmäki WWTP, Helsinki. The Viikinmäki WWTP receives domestic, industrial and hospital wastewater from approx. 800,000 pe. The treatment process in Viikinmäki wastewater treatment plant is based on an activated sludge method and it has three phases: mechanic, biological and chemical treatment.

Effluent from Sweden were sampled at Henriksdal, WWTP, receiving waste water from up to 1 million p.e. The treatment process at Henriksdal wastewater treatment plant is based on an activated sludge method and it has three phases: mechanic, biological and chemical treatment.

Effluent from Greenland was sampled at a sewage drain at Kakillarnat in the northern part of Nuuk. The wastewater is not treated and is mainly domestic and some industrial waste water.

Effluent from Island was sampled at the Klettagardar WWTP. The waste water is treated mechanically and is domestic, industrial, and hospital waste water.

The effluent sample from Norway were taken at VEAS, WWTP, Asker receiving waste water from up to 700,000 p.e. The treatment process at VEAS wastewater treatment plant is based on an activated sludge method and it has three phases: mechanic, biological and chemical treatment.

Table 2: Waste water lines used where effluent samples were taken

Sample ident.	Location	Site	Water (m ³ /year)	Population
FO-1-Eff	Torshavn	UA 11 (Sersjantviken)		11 600
DK-1-Eff	Aarhus	Marselisborg WWTP	10 Million	202 000
FI-1-Eff	Helsinki	Viikinmäki	101 Million	800 000
SE-1-Eff	Stockholm	Henriksdal WWTP	90 Million	1 000 000
GL-1-Eff	Nuuk	Kakillarnat	n.a.	5 000
IS-1-Eff	Reykjavik	Klettagardar WWT	1 Million	100 000
NO-1-Eff	Oslo	VEAS	107 Million	700 000

2.2 Chemical Laboratory Work

For “traditional” target analysis the chemical work is often extremely specialized. Extraction and cleanup methods are optimized towards a small group of compounds. The mass spectrometer used for identification and quantification is normally set to the Selected Ion Monitoring mode (SIM). This gives optimal sensitivity, however, only signals from the target compounds are registered and signals from other compounds are not registered at all. For non-target analysis it is necessary to open up for different compound groups, and more general extraction and cleanup methods are chosen. In addition, the mass spectrometer is set to full scan mode, which means that it registers all mass signals in a given range (see also figure 3, page 21). This non-specialized approach leads to the following limitations: Many compounds, which easily could be detected by a dedicated target method, will be masked or lost either by (1) interfering matrix, (2) instrumental overload/saturation, and (3) possible loss of compounds. Furthermore, the applied GC/LC methods are often not optimal for each single analyte.

For this study a generic extraction and clean-up of samples was carried out at NIVA, Oslo, Norway. All samples were sent to NIVA and stored in freezer at -20 °C before extraction. To cover a broadest possible range of compound groups two different extraction and clean-up methods were applied. The first method is optimized for non-polar and very lipophilic compounds like PCBs, PAHs and other classical POPs, and the second is optimized for polar compounds like pharmaceuticals, modern pesticides and biocides, PFAS, and bisphenols. Prior to extraction, samples were spiked with a number of isotopically labelled internal standards. The final extracts were sent to the different laboratories of the project group.

2.2.1 Sample extraction and clean-up

A mix of deuterated and ^{13}C -labelled pharmaceuticals, bisphenols, PFCs, and BFRs were used as an internal standard for all samples matrices and added before extraction.

Effluent water

Samples of effluent water were filtrated on Spin-X filters and extracted on Oasis HLB (200 mg) solid phase extraction cartridges. After washing the cartridge with MilliQ water and MilliQ water with 5% methanol, the analytes were eluted with 2% formic acid in methanol, methanol, and 2% ammonium hydroxide in methanol. Extracts were evaporated under nitrogen and reconstituted in toluene for GC-MS analysis and methanol for LC-MS analysis.

Sediment

Sediment samples were freeze-dried and 2 g dry sediment was extracted twice by ultrasonic extraction with dichloromethane. To remove elemental sulphur (S_8), which would interfere and corrupt MS-detection, activated copper powder was added to the extracts.¹ For GC-MS analysis no further cleaning was applied and the solvent was exchanged to toluene. For LC-MS analysis the solvent was exchanged to acetonitrile, and the extracts were “washed” twice with n-hexane.

Fish

Between 1 and 4 g fish liver was shaken in 1 h and treated in a ultrasonic bath for 30 min in a solution of acetonitrile, milliQ water, and n-hexane. After centrifugation the n-hexane phase and acetonitrile phase were separated. For GC-MS analysis the n-hexane phase was filtered and further cleaned on a GPC-column. For LC-MS analysis the extracts were filtered.

2.2.2 Full scan MS analysis

To cover a broad spectra of different compounds both GC- and LC-MS was applied (see figure 2). The non-target and suspect screening were performed at NILU and NIVA, Norway and UmU, Sweden.

¹ This sulphur removal is not limited to elemental sulphur, and will also remove organic sulfides like diphenyl disulfide and methionine, but not PFOS and other sulfonic acids.

Figure 2: Application range for GC-MS and LC-MS techniques

Source: NILU.

Full scan analysis with GCxGC-HRMS

Prior to analysis, all samples were concentrated to ~150 µL sample volume. The extracts were injected into an Agilent 7890N GC system equipped with a secondary oven and modulator coupled to a Leco high resolution time-of-flight mass spectrometer (GCxGC-HRMS).

The following GC columns were used:

- 1st oven: 30 m Rtx-5MS (250 µm x 0.25 µm) + 1.29 m Rxi-17Sil MS (250 mm x 0.25 µm).
- Modulator: 0.1 m Rxi-17Sil MS, quad jet two stage modulator.
- 2nd oven: 0.56 m Rxi-17Sil MS + 0.4 m uncoated apolar deactivated silica column (Supelco).
- Transferline: 0.6 m uncoated apolar deactivated silica column (Supelco).

GC-MS settings:

- Injection: 1 µL in pulsed splitless mode.
- Carrier gas: Helium at 1 mL/min.
- 1st oven: 90 °C (2 min), 5 °C/min, 300 °C (11 min).
- 2nd oven: 105 °C (2 min), 5 °C/min, 300 °C (14 min).
- Modulator: temperature offset +15 °C, Modulation period 3.5sec (hot pulse 1.19 sec, cold time 0.56 sec).
- Transferline: 325 °C.

- MS: EI positive mode, high resolution, Acquisition rate 150 spectra/sec, mass range m/z 38-600, ion source temperature 250 °C.

Full scan analysis with GC-ECNI-MS

Prior to analysis, all samples were concentrated to ~150 µL sample volume. The extracts were injected into an Agilent 7890N GC system coupled to an Agilent 7200 QToF mass spectrometer operated in electron capture negative ionization mode (GC-ECNI-HRMS).

The following GC-MS parameters were applied:

- 1 µL pulsed split-less injection, 20 psi for 1 min
- 30m x 0.25 mm x 0.25 µm DB5ms-UI
- He 0.8 mL/min, constant flow
- 90 °C (1 min)-4 °C /min-310 °C (2 min)
- ECNI, methane (40% flow)
- 29-1000 amu, 2 Hz
- High-res mode
- MassHunter, Qual analysis

Full scan analysis with LC-HR-QToF in positive ESI-mode

The analytes were separated on an Acquity UPLC (Waters, Norway) using an Acquity BEH C18 column (100 x 2.1 mm, 1.7 µm) (Waters, Norway) with a methanol and water (10 mM ammonium acetate) mobile phase. Gradient elution was from 2% to 99% methanol over a 13-minute program. The UPLC system was connected to a mass spectrometer (Xevo G2S QToF, (Waters, Norway)) operated in positive electrospray ionisation mode.

Full scan analysis with LC-HR-QToF in negative ESI-mode

The analytes were separated on an Agilent 1290 UHPLC using a Waters Acquity HSS T3 column (150 x 2.1 mm, 1.8 µm) with methanol and water mobile phase. Gradient elution was from 0% to 100% methanol over a 25 minutes program. The UPLC system was connected to a mass spectrometer (Agilent 6550 QToF), operated in negative electrospray ionisation mode.

2.2.3 Storage of raw data

Raw data from all analyses in the project (in the format native to the instrument it was obtained) is being stored at NILU datacentre at secured, fully backed up FTP server.

2.3 Compound identification (Post-acquisition Data Treatment)

2.3.1 Peak picking

Both single ion monitoring (SIM) and especially full scan analyses on high resolution mass spectrometers obtain and register an enormous amount of information. A first step of data reduction is the MS-peak picking algorithm (see details in chapter 2.3.4). In this first step of raw data treatment important information of the mass spectrometric peaks as the mass centroid positions of the peaks, their areas under curve and full-width-at-half-maxima are extracted from the raw MS data and stored for further treatment.

2.3.2 Further post-acquisition work

In parallel with the development of the advanced analytical instruments and software, advanced workflows for an efficient data treatment of full-scan high resolution MS and MSMS-data are a subject of a continuous development. The NORMAN network (<http://www.norman-network.net/>), which is the driving force in this development, has initiated an interlaboratory study (ILS) (Schymanski *et al.*, 2015). One of the major outcomes of this ILS was a general consensus to use a workflow protocol proposed by EAWAG (Schymanski *et al.*, 2014) for acquisition and data treatment. A slightly revised version of this workflow is shown in Figure 3.

Figure 3: Chemical laboratory and post-acquisition data treatment workflow in target and suspect/non-target analysis

Source: NILU based on (Schymanski *et al.*, 2015).

Table 3: Important terms in target and suspect/non-target analysis

Term	Explanation
Chemical Laboratory Workflow	Sample extraction, cleanup, MS-acquisition, and raw data storage
Internal standard	Labeled reference standard added before extraction, used for quantification purposes
Specific cleanup	Removal of disturbing sample matrix, specially adapted to a single group of target compounds
Generic cleanup	Removal of disturbing sample matrix, adapted to a wide range of different compounds
SIM MS	Selected ion monitoring: Mass spectrometric data acquisition limited to some selected ions of a limited number of target compounds
Fullscan MS	Continuous mass spectrometric data acquisition over a large mass range
Raw data	MS-data in a format as generated by the GC- or LC-MS containing information on instrumental parameters and recorded intensity, retention time and mass spectra
Postacquisition Data Treatment Workflow	Data treatment performed on the acquired raw data including peak picking, prioritizing mass spectra of interest, identification steps, and suspect list filtration
Successive non-target identification	Non-target identification starting without prior information from the exact mass, isotope, adduct, and fragmentation information
Suspect list shortcut	Selecting and identifying compounds using prior information as libraries of suspect compounds and other relevant sources
Target shortcut	Identification and normally also quantification by the use of in-house reference compounds
Level 0	Confirmed Structure and Concentration by calibration and internal standard
Level 1	Confirmed Structure by external reference standard
Level 2	Probable Structure by library/diagnostic evidence
Level 3	Tentative Candidate(s) suspect, substructure, class
Level 4	Unequivocal Molecular Formula insufficient structural evidence
Level 5	Mass Spectra of Interest multiple detection, trends etc.

2.3.3 Target analysis

As shown in figure 3 target analysis can be performed in two different ways, either (1) with a traditional approach applying dedicated extraction and cleanup and dedicated mass spectrometry based on single ion monitoring method, or (2) with new combined approach applying more general extraction and cleanup and full scan mass spectrometry. For the time being the traditional approach is still giving better sensitivity and much better control of analytical quality.

The most advanced target methods as dioxin or PCB analysis are normally ending up at confidence level 0 (Confirmed structure and concentration) as shown the above scheme (table 3). However, in some cases target analysis can also end up in Level 1 or Level 2 results. Level 0 or *Confirmed structure and concentration* is close to an ideal situation. Here the proposed structure can be confirmed by correlation to a reference standard with MS, MS/MS and retention time matching and calibration with reference and internal standards for quantification.

The following quality criteria were normally used to ensure correct identification and quantification of the target compound:

- The retention times should match those of the standard compounds within ± 0.1 min.
- The signal-noise ratios are greater than 3:1.
- When a target compound is present in both blank and real samples, it will be reported only if the concentration in the sample is 10 times higher than in the blank.
- Mass error <5ppm.
- MS (/MS) spectra matches up MS (/MS) spectra of pure analytical standards.
- Use of internal standards for measurement of recovery in each single sample and calibration standards for calculation of targeted analyte concentrations.
- For each sample type laboratory blanks followed the sample preparation and quantification procedure as the regular samples to assess background interferences and possible contamination of the samples.

Quantification of target compounds is based on comparison of the compound's peak area to a calibration curve, which is generated in separate runs by injection of calibration solutions of a pure analytical standard of this compound. An internal standard is added in a known amount to the sample and the calibration standards. This standard is used for calibration by calculating the ratio of the signals of the analyte to the internal standard. With this approach loss of the analyte during sample preparation and injection is automatically compensated. The internal standard is a compound that is very similar, but not completely identical to the analyte in the samples, and it is presumed that the internal standard(s) behave like the analyte(s). For isotopically labeled internal standards this presumption is normally valid, but also other analytical standards can fulfill this requirement.

2.3.4 *Suspect screening*

Non-target identification in the meaning of identification of compounds without any prior information is very tedious and time consuming. Therefore, the next and most efficient step of post acquisition data treatment is normally filtration of the list of mass spectra of interest against libraries of suspect compounds. These libraries are either home-made, from commercial supplies or from the NORMAN network and are the most critical part of the suspect screening approach.

Suspect screening leads directly to level 3 (Tentative candidates), which can be described as a “grey zone”, where evidence exists for possible structure(s), but insufficient information for one exact structure only. In fortunate cases it can also lead directly to level 1&2, which means tentatively identified and maybe even semi-quantified.

In this study instruments from different vendors were used and both data formats and software solutions are slightly different. As a typical example the workflow and details for analysis with LC-HR-QToF in negative ESI-mode are described in detail: Raw data acquired with data dependent acquisition mode was analyzed with Mass Hunter Qualitative analysis software (B.07). In the first step, compounds were extracted from the raw data with molecular feature extractor (MFE) algorithm. “The MFE algorithm is a compound finding technique that locates individual sample components (molecular features), even when chromatograms are complex and compounds are not well resolved. MFE locates ions that are covariant (rise and fall together in abundance) but the analysis is not exclusively based on chromatographic peak information. The algorithm uses the accuracy of the mass measurements to group related ions-related by charge-state envelope, isotopic distribution, and/or the presence of adducts and dimers. It assigns multiple species (ions) that are related to the same neutral molecule (for example, ions representing multiple charge states or adducts of the same neutral molecule) to a single compound that is referred to as a feature. Using this approach, the MFE algorithm can locate multiple compounds within a single chromatographic peak.” (Sana, Roark, Li, Waddell, & Fischer, 2008).

In the next step, elemental compositions (molecular formulas) for the unknowns based on the mass spectral data were derived and a number of suspect lists (commercial from Agilent and NILU-list) and mass spectral libraries (including Agilent PCDLs: Forensic Tox, Pesticides and Water Screening) were searched and matched with information available after treatment of raw data.

As a third step, data obtained after treatment with MFE was exported into an open accessible FOR-IDENT platform (Grosse & Letzel, 2016), where a “molecular screening” workflow was applied and allowed to reveal additional compounds.

Compounds, which also are detected in the related blank samples, are reported only if the peak area ratio between the blank and the sample exceeded a factor of 10.

2.3.5 Non-target screening

As described in the previous chapter, non-target identification in the meaning of identification of compounds without any prior information is very time consuming, and can only be done for selected and highly prioritized signals. The selection of signals for further study and evaluation is not an easy task, since nearly all sample types show a huge amount of signals, which are resulting from compounds of natural origin. Different data filtration or suspect screening methods have been applied.

Non-target screening is equivalent to level 4 and 5 (Molecular formula and exact mass). Level 4, *unequivocal molecular formula* can be reached, when a formula can be unambiguously assigned using the spectral information (e.g., adduct, isotope, and/or fragment information), however, there is not enough information available to propose possible structures. In level 5, *Exact mass (m/z)* can be measured in a sample and be of specific interest for the investigation, but information lacks to assign even a molecular formula.

Non-target data evaluation according to this definition was not part of this study; however, all data are stored on an ftp-server and will be available for further data treatment in future.

3. Results and Discussion

A complete list of all tentatively or fully identified compounds (Level 1–3) is given in the Appendix. All raw data containing information, which can be used for non-target analysis in future is stored on an ftp-server hosted by NILU as described in chapter 2.2.3.

3.1 Results from target and suspect screening

The project group has a huge number of different reference standards available and it was possible to identify and (semi)quantify: Per- and polyfluorinated compounds (PFC), chlorinated and brominated compounds, different flame retardants, bisphenols, polycyclic aromatic compounds (PAC), industrial additives like UV-stabilizers, antioxidants, and plasticizers, and pharmaceuticals and personal care products (PPCP). When identified by GC the concentration was estimated in a semi-quantitative way. However, today it is not yet possible to estimate concentrations, when using LC-MS technology.

3.1.1 Per- and polyfluorinated compounds (PFC)

In table 4 examples of identified PFCs are listed.

Table 4: Examples of identified per- and polyfluorinated compounds (PFC)

Compound/Compound group	CAS	Matrix	Frequency	Country
PFNS	68259-12-1	Fish	2/7	FI, SE
PFHxPA	355-46-4	Effluent	2/7	FI, SE
PFHxA	307-24-4	Effluent	2/7	FI, DK
		Sediment	4/7	FI, SE, NO, FO
PFUnDA	2058-94-8	Fish	4/7	FI, SE, DK, NO
PFOS	1763-23-1	Fish	6/7	FI, SE, DK, IS, NO, GL
		Effluent	7/7	FI, SE, DK, IS, NO, GL, FO
PFNA	375-95-1	Fish	3/7	FI, SE, DK
		Effluent	5/7	FI, SE, DK, NO, FO
4:2 FTMAC	1799-84-4	Effluent	5/7	SE, DK, NO, GL, FO
4:3 Acid	80705-13-1	Fish	2/7	SE, GL
C6/C6-PFPIA	40143-77-9	Sediment	2/7	FI, SE
FOSA	754-91-6	Sediment	1/7	NO
4:2 FTAL	135984-67-7	Sediment	1/7	NO
4:2 FTOH	2043-47-2	Sediment	1/7	NO

Residues of perfluorinated alkyl acids (PFAAs) were found in different matrices, and as expected both perfluoro carboxylic acids (PFCAs) and perfluoro sulfonic acids (PFSAAs) were found frequently. However, also a member of a newer class of PFAAs with a phosphonic acid as hydrophilic group, perfluorohexyl phosphonic acid (PFHxPA), was

tentatively identified in water samples from Sweden and Finland. Perfluorinated phosphonic acids, PFPA, are used as anti-foaming agents in the textile industry, in pesticides and lubricants (registered use in Sweden) (Keml, 2006). Recent study indicates that PFPA likely have high persistence and long-range transport potential (Wang, Cousins, Berger, Hungerbuhler, & Scheringer, 2016). PFHxPA has been reported in surface water from Japan (Zushi *et al.*, 2011), Germany (Llorca *et al.*, 2012), China (Jin, Zhang, Zhu, & Martin, 2015), Canada (D'Eon J *et al.*, 2009), in wastewater treatment plant effluents from Canada (D'Eon J *et al.*, 2009) and Germany (Llorca *et al.*, 2012) and in indoor dust from Canada (De Silva, Allard, Spencer, Webster, & Shoeib, 2012).

In addition, emerging compounds like 4:2 FTMAC (1799-84-4) were identified in five out of seven effluent samples, 4:3 Acid (80705-13-1) in two of seven fish samples, and C6/C6-PFPIA (40143-77-9), FOSA (754-91-6), 4:2 FTAL (135984-67-7), and 4:2 FTOH (2043-47-2) were identified in one or two of the seven sediment samples.

The identified PFCs were measured by LC-MS and no information on concentration exists. It is therefore not possible to evaluate the environmental consequences of these findings. Nevertheless the identified emerging compounds should be further investigated with target methods.

3.1.2 Chlorinated and brominated compounds

A long range of different chlorinated and brominated compounds were frequently detected especially in sediment and fish samples, but also in some water samples as shown in table 5.

Table 5: Examples of identified chlorinated and brominated compounds

Compound/Compound group	CAS	Matrix	Frequency	Country
PFNS	68259-12-1	Fish	2/7	FI, SE
PFHxPA	355-46-4	Effluent	2/7	FI, SE
PFHxA	307-24-4	Effluent	2/7	FI, DK
		Sediment	4/7	FI, SE, NO, FO
PFUnDA	2058-94-8	Fish	4/7	FI, SE, DK, NO
PFOS	1763-23-1	Fish	6/7	FI, SE, DK, IS, NO, GL
		Effluent	7/7	FI, SE, DK, IS, NO, GL, FO
PFNA	375-95-1	Fish	3/7	FI, SE, DK
		Effluent	5/7	FI, SE, DK, NO, FO
4:2 FTMAC	1799-84-4	Effluent	5/7	SE, DK, NO, GL, FO
4:3 Acid	80705-13-1	Fish	2/7	SE, GL
C6/C6-PFPIA	40143-77-9	Sediment	2/7	FI, SE
FOSA	754-91-6	Sediment	1/7	NO
4:2 FTAL	135984-67-7	Sediment	1/7	NO
4:2 FTOH	2043-47-2	Sediment	1/7	NO

Note: ¹⁾ Also detected in the related blank samples, reported only if the threshold between the blank and the sample exceeded 10.

In some sediment and all biota samples PCB was found. The chlorinated phosphorous flame retardant TCPP was detected quite frequently, however, this compound is also detected in the blank samples and the exact environmental concentration remains uncertain.

In the sediment sample from Sweden several chlorinated aromatic compounds were found: 3,4,5-trichlorobenzenamine (634-91-3), 1-chloro-3-isocyanatobenzene (2909-38-8), and dichloro and trichloroaniline (CAS 608-27-5 and 634-91-3). Several substituted aniline derivatives are used in the production of dyes and herbicides (Kahl *et al.*, 2000) and these findings may be related to emissions from industrial processes.

2,4-dibromophenol, 2,4,6-tribromoanisole, and 2,4,6-Tribromophenol were detected in all fish samples (not shown in the table 5, see Appendix tables). Bromophenoles and anisoles can be of both industrial and natural origin (Gribble, 2010). In fish samples from Greenland and Faroe Islands a mixed halogenated compound with 3 bromine and 3 chlorine was detected. The exact molecular formula was not possible to determine, however, there are indications that this compound is a natural halogenated monoterpene. Until now, nearly 5000 naturally produced halogen-containing chemicals have been found (Gribble, 2010). Mixed halogenated monoterpenes have been found in different matrices from the marine food chain. The structure of some of the compounds could be elucidated. Red algae has been identified as a major source of these compounds. Algae bloom events may explain the distribution pattern of this compound.

3.1.3 Bisphenols

As shown in table 6 several new bisphenols were identified in different matrices. There is a growing concern that bisphenol A (BPA) which is being used in plastics, receipts, food packaging and other products might be harmful to human health due to its actions as an endocrine-disrupting chemical (Kitamura *et al.*, 2005). Following opinions of scientists, public and regulators manufacturers have begun to replace bisphenol A from their products with a gradual shift to using bisphenol A analogues in their products. These days two of the analogues – bisphenol S (BPS) and bisphenol F (BPF) have been mostly used as bisphenol A replacements. BPS is used in a variety of applications, for example as a developer in a thermal paper, even in the products marketed as “BPA-free paper” (Liao, Liu, & Kannan, 2012). BPS is also used in some industrial applications like electroplating solvent and as constituent of phenolic resins (Clark, 2000). BPF is used to make epoxy resins and coatings such as tanks and pipe linings, industrial floors, adhesives, coatings and electrical varnishes (Fiege *et al.*, 2000).

Similarly, to the S and F analogues also the other bisphenols are found in polymer materials and can be found in the samples taken in this study.

Table 6: Examples of identified bisphenols

Compound/Compound group	CAS	Matrix	Frequency	Country
Bisphenol A	80-05-7	Sediment	3/7	FO, FI, SE
		Effluent	4/7	FI, IS, GL, FO
Bisphenol S	80-09-1	Effluent	4/7	IS, NO, GL, FO,
		Sediment	1/7	IS
		Fish	2/7	GL, FO
4,4-bisphenol F	620-92-8	Effluent	4/7	FI, SE, IS, NO,
		Sediment	2/7	NO, FO,
Bisphenol E	2081-08-5	Effluent	1/7	DK
Bisphenol AF	1478-61-1	Effluent	2/7	GL,
		Fish	4/7	IS, NO, GL, DK
		Sediment	1/7	FI

3.1.4 Polycyclic aromatic compounds (PAC)

The most prominent compound group identified in sediments are polycyclic aromatic compounds, both the pure hydrocarbons (PAHs: pyrene, phenanthrene, perylene etc.), but also heteroaromatics as benzothiazoles, dibenzofuran, acridine, and thiopenes are found. PACs are both of natural and anthropogenic origin. Typical processes which form PACs, are all forms of incomplete combustion, pyrolysis, and geological transformation of organic material. Prominent sources are smoke, soot, tar, creosote, coal, and other fossil products. PACs are often characterized as unintentional by-products.

Table 7: Examples of identified PACs

Compound/Compound group	CAS	Matrix	Frequency	Country
9-methyl acridine	611-64-3	Effluent	5/7	FI, SE, DK, NO, GL,
Fluoranthene	206-44-0	Sediment	6/7	FI, SE, DK, NO, GL, FO
Pyrene	129-00-0	Sediment	6/7	FI, SE, DK, IS, NO, FO
Benz[b]fluoranthene	205-99-2	Sediment	4/7	FO, FI, SE, DK
Benzothiazole	95-16-9	Sediment	6/7	FI, GL, IS, DK, SE, FO

3.1.5 Other industrial additives like UV-stabilizers, antioxidants and plasticizers

Several industrial additives were found in sediment, water and fish samples. These were for instance phenols, UV-stabilizers, antioxidants, and plasticizers of phthalate-type. Also a benzothiazole compound (2-methylthiobenzothiazole, MTBT, CAS: 615-22-5) was frequently found in all sample types and in high concentrations. 2-Methylthiobenzothiazole is a degradation product of mercaptobenzothiazol (MBT, CAS: 149-30-4), which is used in vulcanization of rubber. MTBT has earlier been detected in other screening studies (Blum *et al.*, 2017) in water and other abiotic samples, however, to our best knowledge not yet in marine biota.

Table 8: Examples of identified industrial additives

Compound/Compound group	CAS	Matrix	Frequency	Country
2-(methylthio)benzothiazole	615-22-5	Water	5/7	FI, SE, DK, IS, FO
		Sediment	2/7	FI, NO
		Biota	3/7	SE, DK, NO

3.1.6 Pharmaceuticals and Personal care products (PPCPs)

By suspect screening a huge number of pharmaceuticals were identified in effluent samples. Many of the identified pharmaceuticals are not only found in effluents from sewage treatment plants (STPs) with basic or no treatment but also in STPs with advanced treatment technologies.

Different personal care products were frequently detected in all sample types. Some selected examples are shown in table 9. Triacetin is used as food additive and as a humectant (attracting moisture) in different applications, especially pharmaceuticals. Paroxypropione (70-70-2), a non-steroidal xeno-estrogen, was found in 5 of 7 fish samples. Paroxypropione has structural similarity to parabens, diethylstilbestrol, and alkylphenols, which all are recognized as xeno-estrogens. Methyl salicylate is a salicylic acid derivative, naturally produced by many species of plants, although nowadays it is industrially produced by esterification of the acid with methanol. At high concentrations, this compound acts as a rubefacient, analgesic, and anti-inflammatory. In low concentrations it is also used as a flavoring agent in chewing gums and mints. Its antimicrobial properties are also used in antiseptic mouthwash. Different UV filters (benzophenones and PBS) were found in sediment and effluents. Galaxolide, a musk compound used in high volumes for example by perfume and cologne manufacturers has frequently been found in effluent and fish samples.

Carvone is a terpenoid that has been frequently found in effluents. The compound itself is found naturally in many essential oils, but is most abundant in the oils from seeds of caraway (*Carum carvi*), spearmint (*Mentha spicata*), and dill (de Carvalho & da Fonseca, 2006). Spearmint gums are major uses of natural spearmint oil, and oils containing carvones are used for air freshening products and in aromatherapy.

Table 9: Examples of identified personal care products

Compound/Compound group	CAS	Matrix	Frequency	Country
Triacetin	102-76-1	Effluent	3/7	SE, IS, NO
		Sediment	2/7	SE, FO,
Methyl salicylate	119-36-8	Fish	1/7 ¹⁾	SE
		Effluent	1/7 ¹⁾	SE, IS
Benzophenone-1	119-61-9	sediment	1/7 ¹⁾	GL,
Benzophenone-4	4065-45-6	Effluent	4/7	FI, SE, DK, NO
Phenylbenzimidazole sulfonic acid (PBS)		Effluent	5/7	FI, SE, DK, NO, FO
Paroxypropione	70-70-2	Fish	5/7	FI, SE, DK, GL, FO
Galaxolide	1222-05-5	Effluent	6/7	FI, SE, DK, NO, GL, FO,
		Fish	4/7	SE, IS, NO, FO
Carvone	99-49-0	Effluent	5/7	FI, SE, IS, GL, FO

Note: ¹⁾ Also detected in the related blank samples, reported only if the threshold between the blank and the sample exceeded 10.

3.2 Comparison of effluent water concentrations

The effluent water samples are similar enough to allow a comparison of contaminant levels. Table 10 summarizes the results of the effluent analyses of the most frequently detected compounds (found in at least three effluents). Because the measurements were semi-quantitative in nature, the table only include the maximum concentration of each contaminant (and that value should be regarded as indications only). The focus of the comparison is on the relative concentrations between sewage treatment plants (STP), which should be more reliable.

The STPs are ordered according to the total concentration detected. It is clear that the levels in the effluent is higher for the STPs with less advanced sewage treatment, as in FO, IS and GL. In most cases the highest contaminant concentration was found in effluent from IS or GL. However, for a number of contaminants like m-Cresol, 2-(Methylthio)pyridine, 2-(Methylthio)benzothiazole, 9-methylacridine, 3,3-Diphenylacrylonitrile, 3,3-Diphenylpropionitrile, N-butyl-benzenesulfonamide, and Diclofenac the levels were highest in effluent from one of the STPs in SE, DK or FI, likely because of higher load from industry, traffic and other urban sources.

The concentrations in effluents from STPs with advanced sewage treatment (SE, DK, FI, NO) vs. STPs with basic or no treatment (FO, IS, GL) is likely to reflect the relative persistency of relatively water soluble contaminants. The terpenoids coumarin, carvone, menthol and tetrahydralinalol and the alkaloid caffeine are, for instance, much less abundant in effluent from STPs with advanced treatment. It is plausible that those are degraded in the activated sludge process. Caffeine is known to be easily degraded in active sludge processes (ca 99% removal).

Table 10: Comparison of effluent concentrations of frequently detected compounds (n: 3–7). The individual concentrations have been normalized to 100%, i.e. to the sample with the highest (max) concentration (grey background), and given as relative (percent) concentrations

Name	CAS	Max (µg/L)	SE %	DK %	FI %	NO %	FO %	IS %	GL %	Potential source(s)
m-Cresol	108-39-4	0.2	100	-	-	24	-	-	94	Misc.
N-Formylmorpholine	4394-85-8	0.06	17	-	39	-	-	100	-	Misc.
2-(Methylthio)pyridine	18438-38-5	0.06	33	100	14	66	-	-	-	Misc.
2-Hydroxy acetophenone	582-24-1	30	0.2	0.3	0.4	1	0.3	100	0.1	Misc.
2-Phenoxyethanol	122-99-6	50	0.3	0.2	0.2	-	12	12	100	Misc.
Coumarin	91-64-5	0.08	-	-	-	-	30	100	85	Fragrance, flavour
Carvone	99-49-0	0.3	13	-	16	-	100	62	55	Fragrance, flavour
Menthol	15356-70-4	6	-	-	-	-	47	54	100	Fragrance, flavour
Tetrahydralinalol	78-69-3	4	-	-	-	-	26	25	100	Fragrance, flavour
Dimethyl adipate	627-93-0	0.2	13	-	12	31	-	100	29	Plasticizer
2-(Methylthio) benzothiazole	615-22-5	0.2	53	76	100	-	22	53	-	Rubber
Benzophenone	119-61-9	0.4	26	25	33	61	18	78	100	PPCP
Dipropylene glycol, butyl ether	29911-28-2	4	0.4	-	-	62	5	100	24	Insecticide, solvent
9-methylacridine	611-64-3	1	18	30	100	18	-	-	74	Dyes
Caffeine	58-08-2	30	0.2	0.2	0.2	2	9	99	100	Coffee, pharma
4-Chloro-2-methyl-1-phenyl-3-Buten-1-ol	-	0.1	26	-	35	-	-	-	100	Unknown
2-Methyl-1-Benzyloxybenzene	19578-70-2	7	1	-	2	2	-	100	3	Unknown
3,3-Diphenylacrylonitrile	3531-24-6	0.04	-	100	32	61	-	-	-	Org. synthesis
3,3-Diphenylpropionitrile	2286-54-6	1	22	100	40	6	-	6	-	Org. synthesis
N-butyl-benzenesulfonamide	3622-84-2	0.1	-	100	-	38	-	-	53	Plasticizer
Triacetin	102-76-1	0.2	31	-	32	50	-	100	-	Plasticizer
Galaxolide	1222-05-5	3	13	8	8	13	9	-	100	Fragrance, flavour
Undecyl benzoate	6316-30-9	1	7	4	5	8	5	21	100	PPCP
Diclofenac	15362-40-0	0.2	46	31	100	-	-	-	-	Pharma
Myristyl benzoate	68411-27-8	2	5	4	5	6	4	20	100	PPCP
TCPP	13674-84-5	1	17	23	44	-	-	-	100	Flame retardant
Pentadecyl benzoate	68411-27-8	0.7	9	6	0	11	5	29	100	PPCP

4. Conclusions

With an initial suspect data treatment using different mass spectral data bases it was possible to detect and identify a surprisingly long list of emerging compounds with a level of confidence of three or better. This list is including per- and polyfluorinated compounds (PFC), chlorinated and brominated compounds, flame retardants, bisphenols, polycyclic aromatic compounds (PAC), industrial additives, and pharmaceuticals and personal care products (PPCPs).

When evaluating the total outcome of this study, it is important to keep the following limitations in mind: in order to get a wide overview over all anthropogenic compounds in environmental samples, a general sample preparation method has to be chosen. Many compounds, which easily could be detected by a dedicated target method, will be masked or lost either by (1) interfering matrix, (2) instrumental overload/saturation, and (3) possible loss of compounds. Furthermore, the applied GC/LC methods are often not optimal for each single analyte. For the time being, suspect/non-target cannot replace dedicated target methods in sensitivity and specificity, but proves to be an important tool for identification of compounds of emerging concern.

Non-target identification in the meaning of identification of compounds without any prior information was not part of this study. However, raw data will be stored and made available for retrospective studies. New data treatment tools for real non-target work are under development among several members of the NORMAN network. It has become possible to identify new compounds due to gradients as for instance (1) increasing dilution with growing distance from sources (spatial gradient) (Alygizakis, Oswald, Thomaidis, & Slobodnik, 2016) or (2) increasing bioaccumulation throughout a food chain (Thomas *et al.*, 2015). The project group strongly recommend taking advantage of the extensive knowledge of the NORMAN network and the NORMAN Working group on Non-target screening especially in the phase of selecting sample types and locations.

5. Acknowledgements

5.1 Denmark

Thanks to Anna Gade Holm and Lisbeth Nielsen, Danish Environmental Agency for assistance with selection and collection of samples of effluent and sludge from the waste water treatment plants. Thanks to Jakob Strand and Martin M. Larsen, Institut for Bioscience, Aarhus University for assistance with selection and collection of samples of sediment and fish from marine areas.

5.2 Faroe Islands

The sampling in Álakeri, at the outlet of the Main Hospital sewage treatment plant, demanded some extraordinary sampling crew, and the assistance of the professional divers students at FaroeDive diving school in September 2015 are gratefully acknowledged. So is the assistance of the crew at the SAR vessel Lív who took part in the not so successful fishery expedition, and my colleague at the Environment Agency, Suni Petersen who assisted in a fisheries excursion on his boat himself as skipper. Thanks also to Høgni Arnbjarnarson for lending his fishery gear. Thanks are due also to my colleagues Rakul Mortensen and Jóhannis Danielsen who successfully landed a number of coalfish.

5.3 Finland

Thanks to Markku Korhonen, Finnish Environment Institute (SYKE) for coordinating sampling logistics and personnel at the city of Helsinki for providing the samples for this project.

5.4 Greenland

All Greenlandic samples were collected by Greenland Institute of Natural Resources.

5.5 Iceland

Thanks to Halldór Pálmar Halldórsson from The Sudurnes research center of the University of Iceland for assisting with taking samples to this project.

5.6 Norway

Thanks to Sigurd Øxnevad and Kevin Thomas from The Norwegian Institute for Water Research (NIVA) for delivering the Norwegian samples to this project.

5.7 Sweden

The collection of Swedish samples was coordinated by IVL Swedish Environmental Research Institute.

References

- Alygizakis, N. A., Oswald, P., Thomaidis, N. S., & Slobodnik, J. (2016). *Exploring the Extent of Chemical Pollution Transfer from the Danube River to Black Sea*.
- Blum, K. M., Andersson, P. L., Renman, G., Ahrens, L., Gros, M., Wiberg, K., & Haglund, P. (2017). Non-target screening and prioritization of potentially persistent, bioaccumulating and toxic domestic wastewater contaminants and their removal in on-site and large-scale sewage treatment plants. *Sci Total Environ*, 575, 265-275. <https://doi.org/10.1016/j.scitotenv.2016.09.135>
- Clark, E. (2000). Sulfolane and Sulfones *Kirk-Othmer Encyclopedia of Chemical Technology*: John Wiley & Sons, Inc.
- D'Eon J, C., Crozier, P. W., Furdui, V. I., Reiner, E. J., Libelo, E. L., & Mabury, S. A. (2009). Perfluorinated phosphonic acids in Canadian surface waters and wastewater treatment plant effluent: discovery of a new class of perfluorinated acids. *Environ Toxicol Chem*, 28(10), 2101-2107. <https://doi.org/10.1897/09-048.1>
- de Carvalho, C. C. R., & da Fonseca, M. M. R. (2006). Carvone: Why and how should one bother to produce this terpene. *Food Chemistry*, 95(3), 413-422. <https://doi.org/10.1016/j.foodchem.2005.01.003>
- De Silva, A. O., Allard, C. N., Spencer, C., Webster, G. M., & Shoeib, M. (2012). Phosphorus-containing fluorinated organics: polyfluoroalkyl phosphoric acid diesters (diPAPs), perfluorophosphonates (PFPA), and perfluorophosphinates (PFPIAs) in residential indoor dust. *Environ Sci Technol*, 46(22), 12575-12582. <https://doi.org/10.1021/es303172p>
- Fiege, H., Voges, H.-W., Hamamoto, T., Umemura, S., Iwata, T., Miki, H. Paulus, W. (2000). Phenol Derivatives *Ullmann's Encyclopedia of Industrial Chemistry*: Wiley-VCH Verlag GmbH & Co. KGaA.
- Gribble, G. W. (2010). *Naturally Occurring Organohalogen Compounds – A Comprehensive Update*. Wien: Springer-Verlag. <https://doi.org/10.1007/978-3-211-99323-1>
- Grosse, S., & Letzel, T. (2016). *User Manual for FOR-IDENT Database* (pp. 29).
- Jin, H., Zhang, Y., Zhu, L., & Martin, J. W. (2015). Isomer profiles of perfluoroalkyl substances in water and soil surrounding a chinese fluorochemical manufacturing park. *Environ Sci Technol*, 49(8), 4946-4954. <https://doi.org/10.1021/acs.est.5b00212>
- Kahl, T., Schröder, K.-W., Lawrence, F. R., Marshall, W. J., Höke, H., & Jäckh, R. (2000). Aniline *Ullmann's Encyclopedia of Industrial Chemistry*: Wiley-VCH Verlag GmbH & Co. KGaA.
- Kaj, L., Wallberg, P., & Brorström-Lundén, E. (2014). *Quaternary ammonium compounds – Analyses in a Nordic cooperation on screening*. Retrieved from Copenhagen:
- Keml, S. C. A. (2006). *Perfluorinated substances and their uses in Sweden*. Retrieved from
- Kitamura, S., Suzuki, T., Sanoh, S., Kohta, R., Jinno, N., Sugihara, K. Ohta, S. (2005). Comparative study of the endocrine-disrupting activity of bisphenol A and 19 related compounds. *Toxicol Sci*, 84(2), 249-259. <https://doi.org/10.1093/toxsci/kfi074>
- Liao, C., Liu, F., & Kannan, K. (2012). Bisphenol s, a new bisphenol analogue, in paper products and currency bills and its association with bisphenol a residues. *Environ Sci Technol*, 46(12), 6515-6522. <https://doi.org/10.1021/es300876n>
- Llorca, M., Farre, M., Pico, Y., Muller, J., Knepper, T. P., & Barcelo, D. (2012). Analysis of perfluoroalkyl substances in waters from Germany and Spain. *Science of The Total Environment*, 431, 139-150. <https://doi.org/10.1016/j.scitotenv.2012.05.011>
- Sana, T. R., Roark, J. C., Li, X., Waddell, K., & Fischer, S. M. (2008). Molecular formula and METLIN Personal Metabolite Database matching applied to the identification of compounds generated by LC/TOF-MS. *J Biomol Tech*, 19(4), 258-266.

- Schymanski, E. L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H. P., & Hollender, J. (2014). Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. *Environmental Science & Technology*, 48(4), 2097-2098. <https://doi.org/10.1021/es5002105>
- Schymanski, E. L., Singer, H. P., Slobodnik, J., Ipolyi, I. M., Oswald, P., Krauss, M. Hollender, J. (2015). Non-target screening with high resolution mass spectrometry: Critical review using a collaborative trial on water analysis. *Anal Bioanal Chem*, (accepted). <https://doi.org/10.1007/s00216-015-8681-7>
- Thomas, K. V., Schlabach, M., Langford, K., Reid, M., Fjeld, E., Øxnevad, S. Borgen, A. (2015). *Screening programme 2014: Phosphites, selected PBT substances and non-target screening* (33/2015). Retrieved from Oslo/Kjeller:
- Wang, Z., Cousins, I. T., Berger, U., Hungerbühler, K., & Scheringer, M. (2016). Comparative assessment of the environmental hazards of and exposure to perfluoroalkyl phosphonic and phosphinic acids (PFPA and PFPiAs): Current knowledge, gaps, challenges and research needs. *Environ Int*, 89-90, 235-247. <https://doi.org/10.1016/j.envint.2016.01.023>
- Zushi, Y., Ye, F., Motegi, M., Nojiri, K., Hosono, S., Suzuki, T. Masunaga, S. (2011). Spatially detailed survey on pollution by multiple perfluorinated compounds in the Tokyo Bay basin of Japan. *Environ Sci Technol*, 45(7), 2887-2893. <https://doi.org/10.1021/es103917r>

Sammendrag

På oppdrag fra Nordisk Ministerråd representert av Nordisk kjemikaliegruppe og Havgruppen (HAV) gjennomførte NILU-Norsk Institutt for Luftforskning, Norsk Institutt for Vannforskning (NIVA) og Universitet Umeå-Kemiska institutionen en suspect screening studie som omfattet utløpsvann fra renseanlegg, sediment og fiskeprøver fra alle sju nordiske land.

Denne studien var opprinnelig planlagt som non-target screening, men fagfeltet er under rivende utvikling og stadig nye databearbeidingsrutiner blir utviklet. Dette medfører at man nå skiller strengere mellom de forskjellige konseptene og «suspect screening» har kommet opp som et nytt begrep eller konsept. Det tidligere begrepet non target screening er nå erstattet av suspect screening som baserer seg på omfattende bruk av MS-biblioteker, mens non-target screening kun brukes for dataevaluering av stoffer som man ikke finner i biblioteker.

Hvert av de deltagende land var selv ansvarlig for prøveutvalg, innsamling og forsendelse til analyselaboratoriene som fulgte et på forhånd utarbeidet felles prøvetakingsprotokoll. I hvert land ble det tatt en prøve av utløpsvann fra et stort kommunalt avløpsverk, en sedimentprøve og en fiskeprøve. Vann og sedimentprøver ble tatt som stikkprøver, mens fiskeprøvene var samleprøver av flere individer av samme art. Med unntak av i Danmark ble alle sediment og fiskeprøver tatt i nærhet av vannutløpet. Alle innsamlete prøver ble sent til NIVA, Oslo, Norge for lagring og opparbeidelse. For ikke å fjerne potensielt interessante stoffer ble det valgt to veldig generelle og omfattende ekstraksjons- og opparbeidelsesprosedyrer. Den første var tilpasset og optimalisert for ikke-polare og veldig lipofile forbindelser som PCB, PAH og andre klassiske POPer, mens den andre var optimalisert for mer polare komponenter slik som medisiner, moderne pesticider og biocider, PFAS og bisfenoler. Før starten ble det tilsatt et utvalg isotopmarkerte standarder for å kontrollere opparbeidelsen og for bruk i kvantifiseringen. De ferdige ekstraktene ble sendt til de forskjellige laboratorier i prosjektgruppen.

For å dekke et størst mulig spenn av forskjellige stoffer ble både GC- og LC-MS teknikker brukt (1. GCxGC-HRMS, 2. GC-ECNI-HRMS, 3. LC-QToFMS ESI+, and 4. LC-QToFMS ESI-). Rådata fra alle analyser i prosjektet er lagret på NILUs FTP-server, og er tilgjengelig også for andre forskere i feltet. Som første trinn i databearbeidingen ble de opprinnelige høyoppløste massespektrometriske signaler redusert til retensjonstid, centroid posisjon, areal av signalet og bredde ved halv høyde. Neste og viktigste trinn i suspect screening er en filtrering av alle signaler mot en eller flere databaser med lagrete massespektra av potensielt interessante forbindelser (suspect list). Disse databasene er både laget av instituttene selv, anskaffet fra kommersielle aktører og delt via NORMAN-nettverket. Kvalitet og innhold i databasene er avgjørende for utfallet av dette trinnet. Suspect screening prosedyren leder direkte til en liste av

potensielle kandidatstoffer hvor man har gode indikasjoner, men ikke endelig sikkerhet for den eksakte strukturen.

Følgende stoffgrupper var det mulig å identifisere og delvis også kvantifisere: Per- og polyfluorerte stoffer (PFC), diverse klorerte og bromerte forbindelser, forskjellige flammehemmere, bisfenoler, polysykliske aromatiske forbindelser (PAC), industrielle additiver som UV-stabilisatorer, antioksidanter og mykgjørere, samt legemidler og personlige pleieprodukter (PPCP). For stoffer som ble identifisert ved GC-MS var det mulig å estimere en omtrentlig konsentrasjon. Når det gjelder LC-MS teknikk, er dette foreløpig ikke mulig,

Følgende stoffer kan være relevant for en videre oppfølging:

- I tillegg til mange kjente PFAS forbindelser ble følgende «nye» forbindelser påvist i sedimentprøver: 4:2 FTMAC (1799-84-4), 4:3 Acid (80705-13-1), C6/C6-PFPIA (40143-77-9), FOSA (754-91-6), 4:2 FTAL (135984-67-7), og 4:2 FTOH (2043-47-2).

I den svenske sedimentprøven ble de funnet flere klorerte aromatiske forbindelser: 3,4,5-triklorbenzenamin (634-91-3), 1-kloro-3-isocyanatobenzen (2909-38-8), samt diklor og trikloranilin (CAS 608-27-5 and 634-91-3). Anilinderivater blir brukt i produksjon av fargestoffer og herbicider og kan stamme fra utslipp ved industriell produksjon av disse stoffene, men det kan heller ikke utelukkes at det er nedbrytningsprodukter av disse stoffene.

Det ble påvist flere nye bisfenoler. Det er grunn til bekymring at blant annet bisfenol S, E og AF er påvist i fiskeprøver.

Noen industrielle additiver som fenoler, UV-stabilisatorer, antioksidanter og mykgjørere ble funnet i alle prøvetypene. En grunn til bekymring er funnet av 2-metyltiobenzotiazol (MTBT, CAS: 615-22-5) i fiskeprøvene. Stoffet som brukes i vulkanisering av gummi, er ved tidligere screening studier påvist i utslippsvann og sediment, men dette er, så vidt vi vet, første funnet i biologiske prøver.

Ikke veldig overraskende ble det funnet veldig mange legemidler i prøver av avløpsvann. Men det er grunn til bekymring at mange av legemidlene ikke bare finnes i avløp fra avløpsanlegg med begrenset rensing, men også i avløp fra anlegg med avansert renseteknologi. En sammenligning av kontaminering av avløp fra avanserte rensesanlegg (SE, DK, FI, NO) og anlegg med enkel/ikke rensing (FO, IS, GL) gir informasjon om stoffenes relative persistens. For eksempel finns det mye mindre av terpenoidene kumarin, karvon, mentol og tetrahydrolinalol samt alkaloiden koffein og det antas at disse stoffene nedbrytes i den aktiverte slamprosessen. På den andre siden viser stoffer som m-kresol, 2-(metyltio)pyridin, 2-(metyltio)benzotiazol, 9-metylakridin, 3,3'-difenyllakrylonitril, 3,3'-difenypropionitril, N-butyl-benzensulfonamid, og diclofenac en mye høyere konsentrasjon i avløpsprøver fra SE, DK og FI, trolig på grunn av mye høyere tilførsel fra industri, trafikk og andre urbane kilder.

Med en innledende «suspect» databehandling som bruker forskjellige massespektroskopiske databanker, var det mulig å identifisere en forbausende lang liste av nye miljøgifter med et konfidensnivå på tre eller bedre. Når man vurderer hele resultatet av denne studien er det viktig å ta hensyn til disse begrensningene: for å få en

bredest mulig oversikt over alle antropogene stoffer i miljøprøvene, valgte man en veldig lite spesifikk prøveforberedelse (ekstraksjon og opparbeidelse). Mange stoffer som ellers er lett å detektere med en «target» metode er enten skjult eller blitt borte på grunn av (1) interfererende matriks, (2) overbelastning eller metning av analyseinstrumentet og/eller (3) tap av stoffene under opparbeidelse. Per i dag kan «suspect/non-target screening» ikke erstatte en «target» analyse verken når det gjelder følsomhet eller spesifisitet, men «suspect/non-target screening» er uten tvil blitt et av de viktigste verktøy for identifikasjon av stoffer som kan gi anledning til bekymring for helse eller miljø.

Appendix

Table 11: Effluent Finland

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
2000,23	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
1203,17	C21H44O2Si	18748-91-9	Octadecanoic acid, trimethylsilyl ester	4	2
1058,63	C14H11N	611-64-3	Acridine, 9-methyl-	5	2
703,39	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	2	2
513,86	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	4	2
508,11	C15H13N	2286-54-6	Benzenepropanenitrile, á-phenyl-	5	2
264,64	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
212,42	C18H26O	1222-05-5	Galaxolide	6	2
192,61	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	5	2
189,64	C14H9Cl2NO	15362-40-0	2H-Indol-2-one, 1-(2,6-dichlorophenyl)-1,3-dihydro-	3	3
136,53	C8H6O2	1074-12-0	Phenyglyoxal	6	2
131,81	C12H10O	93-08-3	2-Naphthyl methyl ketone	1	2
130,53	C13H10O	119-61-9	Benzophenone	7	2
129,48	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	6	2
127,05	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
104,95	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
101,37	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
88,82	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
83,84	C20H32O2	-	Benzoic acid, tridecyl ester	7	3
73,23	C9H14O6	102-76-1	Triacetin	4	2
68,99	C12H12O	7228-47-9	à-Methyl-2-naphthalenemethanol	1	2
59,83	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	7	3
47,36	C8H10N4O2	58-08-2	Caffeine	7	3
44,51	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	4	2
43,64	C11H13ClO	-	3-Buten-1-ol, 4-chloro-2-methyl-1-phenyl-	3	2
43,08	C10H14O	99-49-0	Carvone	5	2
24,10	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1	2
23,04	C5H9NO2	4394-85-8	N-Formylmorpholine	3	2
20,83	C15H11N	3531-24-6	2-Propenenitrile, 3,3-diphenyl-	3	2
20,81	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	5	2
19,34	C8H14O4	627-93-0	Hexanedioic acid, dimethyl ester	5	3
13,44	C6H7NS	18438-38-5	Pyridine, 2-(methylthio)-	4	2
	C18H28N2O4		Acebutolol	3	2
	C20H23N		Amitriptyline	6	2
	C20H25ClN2O5		Amlodipine	6	2
	C38H52N6O7		Atazanavir	5	2
	C14H22N2O3		Atenolol	7	2
	C38H72N2O12		Azithromycin	6	2
	C16H19NO4		Benzoyllecgonine	5	2
	C18H31NO4		Bisoprolol	4	2
	C8H10N4O2		Caffeine	7	2
	C15H12N2O		Carbamazepine	7	2
	C15H14N2O3		Carbamazepine, 10, 11-dihydroxy	7	2
	C15H14N2O2		Carbamazepine, 10-hydroxy	7	2
	C20H33N3O4		Celiprolol	4	2
	C21H25ClN2O3		Cetirizine	7	2
	C17H18FN3O3		Ciprofloxacin	7	2
	C19H19FN2O		Citalopram, Desmethyl	4	2
	C20H21FN2O		Citalopram/Escitalopram	7	2
	C38H69NO13		Clarithromycin	6	2
	C18H19ClN4		Clozapine	7	2
	C17H17ClN4		Clozapine, Desmethyl	6	2
	C17H21NO4		Cocaine	5	2
	C18H21NO3		Codeine	6	2
	C10H12N2O		Cotinine	7	2

Continued					
Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₂₂ H ₂₆ N ₂ O ₄ S		Diltiazem	6	2
	C ₂₄ H ₄₀ N ₈ O ₄		Dipyridamol	4	2
	C ₂₃ H ₂₄ N ₂ O ₄ S		Eprosartan	3	2
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₁₇ H ₂₀ F ₆ N ₂ O ₃		Flecainide	5	2
	C ₁₈ H ₂₁ NO ₃		Hydrocodone	6	2
	C ₂₅ H ₂₈ N ₆ O		Irbesartan	4	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2
	C ₂₀ H ₂₃ N		Maprotiline	6	2
	C ₁₁ H ₁₅ NO ₂		MDMA	5	2
	C ₂₁ H ₂₇ NO		Methadone	4	2
	C ₁₄ H ₂₂ ClN ₃ O ₂		Metoclopramide	6	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2
	C ₁₅ H ₁₁ ClN ₂ O ₂		Oxazepam	6	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₆ H ₁₅ F ₆ N ₅ O		Sitagliptin	5	2
	C ₁₂ H ₂₀ N ₂ O ₃ S		Sotalol	6	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	7	2
	C ₁₅ H ₂₃ N ₃ O ₄ S		Sulpiride	4	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	5	2
	C ₃₃ H ₃₀ N ₄ O ₂		Telmisartan	6	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	7	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	8	2
	C ₂₄ H ₂₉ N ₅ O ₃		Valsartan	5	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	7	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine,-O-demethyl-	7	2
	C ₁₇ H ₂₀ N ₄ S	132539-06-1	OLANZAPINE	1	3
	C ₁₀ H ₁₂ N ₄ O ₅	58-63-9	Inosine	1	3
	C ₁₃ H ₁₃ N ₃ O ₃ S	19077-98-6	N-Acetylsulfapyridin	2	3
	C ₇ H ₈ ClN ₃ O ₄ S ₂	58-93-5	HYDROCHLOROTHIAZIDE	5	3
	C ₁₂ H ₂₆ O ₄ S	4706-78-9	dodecyl sulfuric acid	3	3
	C ₁₂ H ₁₁ N ₃ O ₃ S	104-23-4	4'-aminoazobenzene-4-sulfonic acid	2	3
	C ₁₃ H ₁₀ N ₂ O ₃ S	27503-81-7	2-phenyl-1H-benzimidazole-5-sulphonic acid	7	3
	C ₁₇ H ₁₉ N ₃ O ₄ S	88546-55-8	Omeprazole Sulfone	1	3
		40143-76-8	PFHxPA	2	3
		2043-47-2	4:2 FTOH	1	3
		620-92-8	4,4'-BPF	4	2
		137862-53-4	Valsartan	3	3
		4065-45-6	benzophenone-4	5	3
		27503-81-7	PBS (Phenylbenzimidazole sulfonic acid)	7	3
		58-93-5	Hydrochlorothiazide	5	3
		123-08-0	4-hydroxybenzaldehyde	7	3

Table 12: Effluent Sweden

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3824,61	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
1102,76	C ₁₀ H ₁₆	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
1046,77	C ₂₁ H ₄₄ O ₂ Si	18748-91-9	Octadecanoic acid, trimethylsilyl ester	4	2
329,05	C ₁₈ H ₂₆ O	1222-05-5	Galaxolide	6	2
297,52	C ₁₈ H ₃₈ O ₂ Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	4	2
273,84	C ₁₅ H ₁₃ N	2286-54-6	Benzenepropanenitrile, á-phenyl-	5	2
203,31	C ₁₇ H ₃₆ O ₂ Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	5	2
201,91	C ₇ H ₈ O	108-39-4	Phenol, 3-methyl-	3	2
198,79	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	4	2
189,35	C ₁₄ H ₁₁ N	611-64-3	Acridine, 9-methyl-	5	2
159,37	C ₈ H ₁₀ O ₂	122-99-6	Ethanol, 2-phenoxy-	6	2
120,70	C ₈ H ₆ O ₂	1074-12-0	Phenylglyoxal	6	2
104,57	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
101,37	C ₈ H ₇ NS ₂	615-22-5	Benzothiazole, 2-(methylthio)-	5	2
92,19	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
88,30	C ₁₄ H ₁₄ O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
86,69	C ₁₄ H ₉ Cl ₂ NO	15362-40-0	2H-Indol-2-one, 1-(2,6-dichlorophenyl)-1,3-dihydro-	3	3
85,51	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	7	3
85,03	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	7	3
76,10	C ₈ H ₈ O ₂	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
69,85	C ₉ H ₁₄ O ₆	102-76-1	Triacetin	4	2
63,63	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
61,76	C ₈ H ₁₀ N ₄ O ₂	58-08-2	Caffeine	7	3
58,09	C ₂₂ H ₃₆ O ₂	-	Benzoic acid, pentadecyl ester	6	3
33,42	C ₁₀ H ₁₄ O	99-49-0	Carvone	5	2
32,81	C ₁₁ H ₁₃ ClO	-	3-Buten-1-ol, 4-chloro-2-methyl-1-phenyl-	3	2
31,21	C ₆ H ₇ NS	18438-38-5	Pyridine, 2-(methylthio)-	4	2
21,19	C ₈ H ₁₄ O ₄	627-93-0	Hexanedioic acid, dimethyl ester	5	3
16,27	C ₇ H ₅ NOS	934-34-9	2(3H)-Benzothiazolone	2	3
14,35	C ₁₀ H ₂₂ O ₃	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	5	3
10,15	C ₅ H ₉ NO ₂	4394-85-8	N-Formylmorpholine	3	2
9,43	C ₁₁ H ₁₀	90-12-0	Naphthalene, 1-methyl-	2	2
	C ₁₈ H ₂₈ N ₂ O ₄		Acebutolol	3	2
	C ₂₀ H ₂₃ N		Amitriptyline	6	2
	C ₂₀ H ₂₅ ClN ₂ O ₅		Amlodipine	6	2
	C ₃₈ H ₅₂ N ₆ O ₇		Atazanavir	5	2
	C ₁₄ H ₂₂ N ₂ O ₃		Atenolol	7	2
	C ₃₈ H ₇₂ N ₂ O ₁₂		Azithromycin	6	2
	C ₁₆ H ₁₉ NO ₄		Benzoyllecgonine	5	2
	C ₁₈ H ₃₁ NO ₄		Bisoprolol	4	2
	C ₈ H ₁₀ N ₄ O ₂		Caffeine	7	2
	C ₁₅ H ₁₂ N ₂ O		Carbamazepine	7	2
	C ₁₅ H ₁₄ N ₂ O ₃		Carbamazepine, 10, 11-dihydroxy	7	2
	C ₁₅ H ₁₄ N ₂ O ₂		Carbamazepine, 10-hydroxy	7	2
	C ₂₀ H ₃₃ N ₃ O ₄		Celiprolol	4	2
	C ₂₁ H ₂₅ ClN ₂ O ₃		Cetirizine	7	2
	C ₁₇ H ₁₈ FN ₃ O ₃		Ciprofloxacin	7	2
	C ₁₉ H ₁₉ FN ₂ O		Citalopram, Desmethyl	4	2
	C ₂₀ H ₂₁ FN ₂ O		Citalopram/Escitalopram	7	2
	C ₃₈ H ₆₉ NO ₁₃		Clarithromycin	6	2
	C ₁₈ H ₁₉ ClN ₄		Clozapine	7	2
	C ₁₇ H ₁₇ ClN ₄		Clozapine, Desmethyl	6	2
	C ₁₇ H ₂₁ NO ₄		Cocaine	5	2
	C ₁₈ H ₂₁ NO ₃		Codeine	6	2
	C ₁₀ H ₁₂ N ₂ O		Cotinine	7	2
	C ₂₂ H ₂₆ N ₂ O ₄ S		Diltiazem	6	2
	C ₂₃ H ₂₄ N ₂ O ₄ S		Eprosartan	3	2
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₁₇ H ₂₀ F ₆ N ₂ O ₃		Flecainide	5	2
	C ₁₈ H ₂₁ NO ₃		Hydrocodone	6	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2

Continued

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₂₀ H ₂₃ N		Maprotiline	6	2
	C ₁₁ H ₁₅ NO ₂		MDMA	5	2
	C ₂₁ H ₂₇ NO		Methadone	4	2
	C ₁₄ H ₂₂ ClN ₃ O ₂		Metoclopramide	6	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2
	C ₁₅ H ₁₁ ClN ₂ O ₂		Oxazepam	6	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₆ H ₁₅ F ₆ N ₅ O		Sitagliptin	5	2
	C ₁₂ H ₂₀ N ₂ O ₃ S		Sotalol	6	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	7	2
	C ₁₅ H ₂₃ N ₃ O ₄ S		Sulpiride	4	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	7	2
	C ₃₃ H ₃₀ N ₄ O ₂		Telmisartan	5	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	6	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	7	2
	C ₂₄ H ₂₉ N ₅ O ₃		Valsartan	8	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	9	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine,-O-demethyl-	7	2
	C ₂₄ H ₄₈ O ₂	13945-76-1	dodecyl dodecanoate	1	2
	C ₂₀ H ₄₀ O ₂	506-30-9	icosanoic acid	2	2
	C ₉ H ₁₉ NO ₄	16485-10-2	panthenol , DL-form	2	2
	C ₁₈ H ₁₄ F ₄ N ₂ O ₄ S		Bicalutamid	3	2
	C ₉ H ₁₁ NO ₂	94-09-7	BENZOCAINE	2	2
	C ₁₁ H ₁₀ N ₄ O ₄	6804-07-5	carbadox	1	2
	C ₆ H ₇ N ₅	1198-47-6	6-Methylthioguanin	1	2
	C ₁₄ H ₉ ClF ₃ NO ₃	205754-32-1	rac 8-Hydroxy Efavirenz	1	2
	C ₁₃ H ₁₃ N ₃ O ₃ S	19077-98-6	N-Acetylsulfapyridin	2	2
	C ₁₄ H ₁₂ O ₆ S	4065-45-6	sulisobenzone	5	2
	C ₅ H ₈ O ₃	105-45-3	methyl acetoacetate	2	2
	C ₁₁ H ₁₁ N ₃ O ₂ S	144-83-2	sulfapyridine	1	2
	C ₂₂ H ₄₃ NO		docos-13-enamide, Amides, C22 (unsaturated)	0	2
	C ₁₃ H ₁₀ N ₂ O ₃ S	27503-81-7	2-phenyl-1H-benzimidazole-5-sulphonic acid	7	2
	C ₈ H ₅ NO ₂	85-41-6	1H-Isoindole-1,3(2H)-dione	2	2
	C ₇ H ₉ NO ₂	30652-11-0	Deferiprone	2	2
	C ₂ HF ₃ O ₂	76-05-1	trifluoroacetic acid	1	2
	C ₆ H ₆ N ₄ O ₂	552-62-5	7-Methylxanthin	1	2
	C ₁₂ H ₁₁ N ₃ O ₃ S	104-23-4	4'-aminoazobenzene-4-sulfonic acid	2	2
	C ₁₈ H ₃₆ O ₂	57-11-4	Octadecanoic acid	2	2
	C ₁₂ H ₂₆ O ₄ S	4706-78-9	dodecyl sulfuric acid	3	2
		1799-84-4	4:2 FTMAC	5	2
		40143-76-8	PFHxPA	2	2
		68259-15-4	MeFHxSA	2	2
		620-92-8	4,4-BPF	4	1
		13595-25-0	bisphenol M	5	1
		79-94-7	tetrabromobisphenol A	1	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		4065-45-6	benzophenone-4 (sulisobenzone)	5	2
		27503-81-7	PBS (Phenylbenzimidazole sulfonic acid)	7	2
		58-93-5	Hydrochlorothiazide	5	2
		90357-06-5	bicalutamide	3	2

Table 13: Effluent Denmark

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/matrix	ID Level
1265,13	C ₁₅ H ₁₃ N	2286-54-6	Benzenepropanenitrile, á-phenyl-	5	2
1250,26	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
319,42	C ₁₄ H ₁₁ N	611-64-3	Acridine, 9-methyl-	5	2
317,09	C ₁₀ H ₁₆	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
284,27	C ₈ H ₆ O ₂	1074-12-0	Phenylglyoxal	6	2
271,02	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	4	2
203,85	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-, 2,4,4-trimethylpentyl ester	7	2
200,60	C ₁₈ H ₂₆ O	1222-05-5	Galaxolide	6	2
177,27	C ₁₀ H ₁₅ NO ₂ S	3622-84-2	Benzenesulfonamide, N-butyl-	3	2
146,93	C ₈ H ₇ NS ₂	615-22-5	Benzothiazole, 2-(methylthio)-	5	2
101,28	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
94,97	C ₈ H ₈ O ₂	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
93,57	C ₆ H ₇ NS	18438-38-5	Pyridine, 2-(methylthio)-	4	2
87,05	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
80,94	C ₈ H ₁₀ O ₂	122-99-6	Ethanol, 2-phenoxy-	6	2
66,76	C ₁₂ H ₁₈ O	2934-05-6	Phenol, 2,4-bis(1-methylethyl)-	1	2
66,06	C ₁₅ H ₁₁ N	3531-24-6	2-Propenenitrile, 3,3-diphenyl-	3	2
58,97	C ₁₄ H ₉ Cl ₂ NO	15362-40-0	2H-Indol-2-one, 1-(2,6-dichlorophenyl)-1,3-dihydro-	3	3
56,11	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	7	3
54,28	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	7	3
47,08	C ₈ H ₁₀ N ₄ O ₂	58-08-2	Caffeine	7	3
39,73	C ₂₂ H ₃₆ O ₂	-	Benzoic acid, pentadecyl ester	6	3
	C ₂₀ H ₂₃ N		Amitriptyline	6	2
	C ₂₀ H ₂₅ ClN ₂ O ₅		Amlodipine	6	2
	C ₃ H ₅ N ₂ O ₇		Atazanavir	5	2
	C ₁₄ H ₂₂ N ₂ O ₃		Atenolol	7	2
	C ₃ H ₇ N ₂ O ₁₂		Azithromycin	6	2
	C ₁₆ H ₁₉ NO ₄		Benzoylcegonine	5	2
	C ₁₈ H ₃₁ NO ₄		Bisoprolol	4	2
	C ₈ H ₁₀ N ₄ O ₂		Caffeine	7	2
	C ₁₅ H ₁₂ N ₂ O		Carbamazepine	7	2
	C ₁₅ H ₁₄ N ₂ O ₃		Carbamazepine, 10, 11-dihydroxy	7	2
	C ₁₅ H ₁₄ N ₂ O ₂		Carbamazepine, 10-hydroxy	7	2
	C ₂₀ H ₃₃ N ₃ O ₄		Celiprolol	4	2
	C ₂₁ H ₂₅ ClN ₂ O ₃		Cetirizine	7	2
	C ₁₇ H ₁₈ FN ₃ O ₃		Ciprofloxacin	7	2
	C ₁₉ H ₁₉ FN ₂ O		Citalopram, Desmethyl	4	2
	C ₂₀ H ₂₁ FN ₂ O		Citalopram/Escitalopram	7	2
	C ₃ H ₆ NO ₁₃		Clarithromycin	6	2
	C ₁₈ H ₁₉ ClN ₄		Clozapine	7	2
	C ₁₇ H ₁₇ ClN ₄		Clozapine, Desmethyl	6	2
	C ₁₇ H ₂₁ NO ₄		Cocaine	5	2
	C ₁₈ H ₂₁ NO ₃		Codeine	6	2
	C ₁₀ H ₁₂ N ₂ O		Cotinine	7	2
	C ₂₂ H ₂₆ N ₂ O ₄ S		Diltiazem	6	2
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₁₇ H ₂₀ F ₆ N ₂ O ₃		Flecainide	5	2
	C ₁₈ H ₂₁ NO ₃		Hydrocodone	6	2
	C ₂₅ H ₂₈ N ₆ O		Irbesartan	4	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2
	C ₂₀ H ₂₃ N		Maprotiline	6	2
	C ₁₁ H ₁₅ NO ₂		MDMA	5	2
	C ₂₁ H ₂₇ NO		Methadone	4	2
	C ₁₄ H ₂₂ ClN ₃ O ₂		Metoclopramide	6	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2
	C ₁₅ H ₁₁ ClN ₂ O ₂		Oxazepam	6	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2

Continued					
Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₆ H ₁₅ F ₆ N ₅ O		Sitagliptin	5	2
	C ₁₂ H ₂₀ N ₂ O ₃ S		Sotalol	6	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	7	2
	C ₁₅ H ₂₃ N ₃ O ₄ S		Sulpiride	4	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	7	2
	C ₃₃ H ₃₀ N ₄ O ₂		Telmisartan	5	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	7	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	7	2
	C ₂₄ H ₂₉ N ₅ O ₃		Valsartan	5	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	7	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine, -O-demethyl-	7	2
	C ₁₂ H ₂₆ O ₄ S	4706-78-9	dodecyl sulfuric acid	3	2
	C ₁₄ H ₃₀ O ₄ S	4754-44-3	tetradecyl sulfate	1	2
	C ₁₈ H ₁₀	27208-37-3	Cyclopenta(c,d)pyren	1	2
	C ₁₃ H ₁₂ F ₂ N ₆ O	86386-73-4	fluconazole	1	2
	C ₉ H ₁₈ O ₂	112-05-0	nonanoic acid	1	2
	C ₉ H ₁₈ O ₂	111-11-5	methyl octanoate	1	2
	C ₉ H ₁₈ O ₂	3302-10-1	3,5,5-trimethylhexanoic acid	1	2
	C ₉ H ₁₈ O ₂	816-19-3	Methyl 2-ethylhexanoate	1	2
	C ₉ H ₁₈ O ₂	59354-78-8	neononanoic acid	1	2
	C ₁₆ H ₃₀ O ₂	68227-33-8	2,5,8,11-tetramethyldodec-6-yne-5,8-diol	1	2
	C ₁₆ H ₃₀ O ₂	142-90-5	dodecyl methacrylate	2	2
	C ₂₀ H ₃₀ O ₂	14507-49-4	13-ethyl-3-methoxygona-2,5(10)-dien-17β-ol	1	2
	C ₂₀ H ₃₀ O ₂	153-00-4	metenolone	1	2
	C ₂₀ H ₃₀ O ₂	58-18-4	17-alpha-Methyltestosterone	1	2
		1799-84-4	4:2 FTMAC	5	2
		13595-25-0	bisphenol M	5	1
		41340-25-4	etodolac (NSAID drug)	1	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		29878-31-7	4-methylbenzotriazole (tolyltriazole)	1	2
		4065-45-6	benzophenone-4 (sulisobenzene)	5	2
		27503-81-7	PBS (Phenylbenzimidazole sulfonic acid)	7	2
		58-93-5	Hydrochlorothiazide	5	2
		90357-06-5	bicalutamide	3	2

Table 14: Effluent Iceland

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/matrix	ID Level
32217,37	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
26445,96	C8H10N4O2	58-08-2	Caffeine	7	3
19931,70	C12H12O5	5062-30-6	Phenacylidene diacetate	1	2
6967,67	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
6129,79	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	6	2
5116,88	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
3939,27	C10H22O3	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	5	3
3373,97	C10H20O	15356-70-4	DL-Menthol	3	2
2256,37	C7H7NO2	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	1	3
2186,77	C8H10O	60-12-8	Phenylethyl Alcohol	2	3
2175,35	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
1118,58	C10H22O	78-69-3	3-Octanol, 3,7-dimethyl-	3	2
732,87	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
732,61	C10H12O2	122-84-9	2-Propanone, 1-(4-methoxyphenyl)-	1	2
589,01	C12H20O2	18679-18-0	2(3H)-Furanone, dihydro-5-(2-octenyl)-, (Z)-	1	2
492,40	C6H6O2	108-46-3	Resorcinol	1	2
376,55	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
357,81	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	5	2
335,31	C7H8O2	504-15-4	Orcinol	1	2
314,70	C20H32O2	-	Benzoic acid, tridecyl ester	7	3
310,39	C13H10O	119-61-9	Benzophenone	7	2
278,29	C10H8	91-20-3	Naphthalene	1	2
277,94	C8H8O2	57295-30-4	3-Hydroxy-4-methylbenzaldehyde	2	3
271,63	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	7	3
265,96	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	4	2
249,69	C10H14	527-53-7	Benzene, 1,2,3,5-tetramethyl-	1	2
225,38	C9H14O6	102-76-1	Triacetin	4	2
213,52	C10H14O	39852-87-4	Tricyclo[5.2.1.0(2,6)]dec-3-en-10-ol	2	3
195,83	C10H22O2	1559-35-9	Ethanol, 2-[(2-ethylhexyl)oxy]-	1	2
193,41	C22H36O2	-	Benzoic acid, pentadecyl ester	6	3
187,42	C8H7NO	2380-94-1	1H-Indol-4-ol	2	3
172,97	C10H14O2Si	2078-12-8	Benzoic acid trimethylsilyl ester	1	2
162,88	C10H14O	99-49-0	Carvone	5	2
161,99	C8H14O4	627-93-0	Hexanedioic acid, dimethyl ester	5	3
155,73	C10H14	488-23-3	Benzene, 1,2,3,4-tetramethyl-	1	2
153,53	C9H10O2	140-11-4	Acetic acid, phenylmethyl ester	1	2
142,14	C21H44O2Si	18748-91-9	Octadecanoic acid, trimethylsilyl ester	4	2
102,41	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	5	2
81,38	C15H13N	2286-54-6	Benzenepropanenitrile, α -phenyl-	5	2
79,00	C9H6O2	91-64-5	Coumarin	3	2
62,66	C13H12	643-93-6	1,1'-Biphenyl, 3-methyl-	1	2
58,71	C5H9NO2	4394-85-8	N-Formylmorpholine	3	2
43,71	C11H10	90-12-0	Naphthalene, 1-methyl-	2	2
	C20H23N		Amitriptyline	6	2
	C20H25ClN2O5		Amlodipine	6	2
	C14H22N2O3		Atenolol	7	2
	C38H72N2O12		Azithromycin	6	2
	C16H19NO4		Benzoylcegonine	5	2
	C8H10N4O2		Caffeine	7	2
	C15H12N2O		Carbamazepine	7	2
	C15H14N2O3		Carbamazepine, 10, 11-dihydroxy	7	2
	C15H14N2O2		Carbamazepine, 10-hydroxy	7	2
	C21H25ClN2O3		Cetirizine	7	2
	C17H18FN3O3		Ciprofloxacin	7	2
	C20H21FN2O		Citalopram/Escitalopram	7	2
	C38H69NO13		Clarithromycin	6	2
	C18H19ClN4		Clozapine	7	2
	C17H17ClN4		Clozapine, Desmethyl	6	2
	C17H21NO4		Cocaine	5	2
	C18H21NO3		Codeine	6	2
	C10H12N2O		Cotinine	7	2
	C22H26N2O4S		Diltiazem	6	2
	C24H40N8O4		Dipyridamol	4	2

Continued

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₁₇ H ₂₀ F ₆ N ₂ O ₃		Flecainide	5	2
	C ₁₈ H ₂₁ NO ₃		Hydrocodone	6	2
	C ₂₅ H ₂₈ N ₆ O		Irbesartan	4	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2
	C ₂₀ H ₂₃ N		Maprotiline	6	2
	C ₁₁ H ₁₅ NO ₂		MDMA	5	2
	C ₁₄ H ₂₂ ClN ₃ O ₂		Metoclopramide	6	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2
	C ₁₅ H ₁₁ ClN ₂ O ₂		Oxazepam	6	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₆ H ₁₅ F ₆ N ₅ O		Sitagliptin	5	2
	C ₁₂ H ₂₀ N ₂ O ₃ S		Sotalol	6	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	8	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	9	2
	C ₃₃ H ₃₀ N ₄ O ₂		Telmisartan	5	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	7	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	7	2
	C ₂₄ H ₂₉ N ₅ O ₃		Valsartan	5	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	7	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine, -O-demethyl-	7	2
	C ₁₅ H ₁₁ ClO ₃	2536-31-4	Chlorflurenol-methyl (ester)	2	2
	C ₆ H ₁₂ O ₆	50-99-7	glucose	1	2
	C ₂₀ H ₄₀ O ₂	506-30-9	icosanoic acid	2	2
	C ₂₉ H ₄₄ O ₁₂	630-60-4	ouabain	1	2
	C ₁₇ H ₃₄ O ₂	6309-51-9	isopentyl laurate	3	2
	C ₁₇ H ₃₄ O ₂	110-27-0	Wickenol 101	3	2
	C ₁₇ H ₃₄ O ₂	112-39-0	methyl palmitate	2	2
	C ₁₆ H ₃₀ O ₂	142-90-5	dodecyl methacrylate	2	2
	C ₁₈ H ₃₆ O ₂	57-11-4	Octadecanoic acid	2	2
	C ₁₆ H ₁₀ ClN ₃ O ₃	2814-77-9	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	2	2
		80-09-1	bisphenol S	3	2
		620-92-8	4,4'-BPF	4	1
		13595-25-0	bisphenol M	5	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		137862-53-4	Valsartan	3	2
		93-35-6	umbelliferone	1	2
		58-93-5	Hydrochlorothiazide	5	2
		103-90-2	paracetamol	5	2

Table 15: Effluent Norway

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
2448,71	C ₁₀ H ₂₂ O ₃	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	5	2
1826,70	C ₁₈ H ₃₉ O ₇ P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	2	2
825,94	C ₁₀ H ₁₆	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	2
644,57	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
541,62	C ₈ H ₁₀ N ₄ O ₂	58-08-2	Caffeine	7	2
338,05	C ₁₈ H ₂₆ O	1222-05-5	Galaxolide	6	2
335,23	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	2
242,90	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
213,55	C ₈ H ₈ O ₂	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
194,79	C ₈ H ₆ O ₂	1074-12-0	Phenylglyoxal	6	3
192,41	C ₁₄ H ₁₁ N	611-64-3	Acridine, 9-methyl-	5	2
134,97	C ₂₁ H ₄₄ O ₂ Si	18748-91-9	Octadecanoic acid, trimethylsilyl ester	4	2
132,98	C ₁₄ H ₁₄ O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	3
113,72	C ₉ H ₁₄ O ₆	102-76-1	Triacetin	4	3
95,44	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	7	3
89,52	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	7	3
80,03	C ₁₅ H ₁₃ N	2286-54-6	Benzenepropanenitrile, α -phenyl-	5	2
77,63	C ₂₂ H ₃₆ O ₂	-	Benzoic acid, pentadecyl ester	6	2
67,64	C ₁₀ H ₁₅ NO ₂ S	3622-84-2	Benzenesulfonamide, N-butyl-	3	2
65,53	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	3
61,76	C ₆ H ₇ NS	18438-38-5	Pyridine, 2-(methylthio)-	4	2
50,79	C ₈ H ₁₄ O ₄	627-93-0	Hexanedioic acid, dimethyl ester	5	2
49,39	C ₇ H ₈ O	108-39-4	Phenol, 3-methyl-	3	3
40,21	C ₁₅ H ₁₁ N	3531-24-6	2-Propenenitrile, 3,3-diphenyl-	3	3
34,02	C ₈ H ₈ O ₂	57295-30-4	3-Hydroxy-4-methylbenzaldehyde	2	3
	C ₁₈ H ₂₈ N ₂ O ₄		Acebutolol	3	2
	C ₂₀ H ₂₃ N		Amitriptyline	6	2
	C ₃₈ H ₅₂ N ₆ O ₇		Atazanavir	5	2
	C ₁₄ H ₂₂ N ₂ O ₃		Atenolol	7	2
	C ₃₈ H ₇₂ N ₂ O ₁₂		Azithromycin	6	2
	C ₁₆ H ₁₉ NO ₄		Benzoyllecgonine	5	2
	C ₁₈ H ₃₁ NO ₄		Bisoprolol	4	2
	C ₈ H ₁₀ N ₄ O ₂		Caffeine	7	2
	C ₁₅ H ₁₂ N ₂ O		Carbamazepine	7	2
	C ₁₅ H ₁₄ N ₂ O ₃		Carbamazepine, 10, 11-dihydroxy	7	2
	C ₁₅ H ₁₄ N ₂ O ₂		Carbamazepine, 10-hydroxy	7	2
	C ₂₀ H ₃₃ N ₃ O ₄		Celiprolol	4	2
	C ₂₁ H ₂₅ ClN ₂ O ₃		Cetirizine	7	2
	C ₁₇ H ₁₈ FN ₃ O ₃		Ciprofloxacin	7	2
	C ₂₀ H ₂₁ FN ₂ O		Citalopram/Escitalopram	7	2
	C ₃₈ H ₆₉ NO ₁₃		Clarithromycin	6	2
	C ₁₈ H ₁₉ ClN ₄		Clozapine	7	2
	C ₁₇ H ₁₇ ClN ₄		Clozapine, Desmethyl	6	2
	C ₁₇ H ₂₁ NO ₄		Cocaine	5	2
	C ₁₈ H ₂₁ NO ₃		Codeine	6	2
	C ₁₀ H ₁₂ N ₂ O		Cotinine	7	2
	C ₂₂ H ₂₆ N ₂ O ₄ S		Diltiazem	6	2
	C ₂₄ H ₄₀ N ₈ O ₄		Dipyridamol	4	2
	C ₂₃ H ₂₄ N ₂ O ₄ S		Eprosartan	3	2
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₁₇ H ₂₀ F ₆ N ₂ O ₃		Flecainide	5	2
	C ₁₈ H ₂₁ NO ₃		Hydrocodone	6	2
	C ₂₅ H ₂₈ N ₆ O		Irbesartan	4	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2
	C ₂₀ H ₂₃ N		Maprotiline	6	2
	C ₁₁ H ₁₅ NO ₂		MDMA	5	2
	C ₂₁ H ₂₇ NO		Methadone	4	2
	C ₁₄ H ₂₂ ClN ₃ O ₂		Metoclopramide	6	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2

Continued

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₁₅ H ₁₁ ClN ₂ O ₂		Oxazepam	6	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₆ H ₁₅ F ₆ N ₅ O		Sitagliptin	5	2
	C ₁₂ H ₂₀ N ₂ O ₃ S		Sotalol	6	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	7	2
	C ₁₅ H ₂₃ N ₃ O ₄ S		Sulpiride	4	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	7	2
	C ₃₃ H ₃₀ N ₄ O ₂		Telmisartan	5	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	7	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	7	2
	C ₂₄ H ₂₉ N ₅ O ₃		Valsartan	5	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	7	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine, -O-demethyl-	7	2
	C ₄ H ₄ N ₂ O ₃	67-52-7	2,4,6-(1H,3H,5H)-Pyrimidinetrione	1	2
	C ₅ H ₈ O ₃	105-45-3	methyl acetoacetate	2	2
	C ₁₇ H ₃₄ O ₂	6309-51-9	isopentyl laurate	3	2
	C ₁₇ H ₃₄ O ₂	110-27-0	Wickenol 101	3	2
	C ₁₅ H ₃₀ O ₂	124-10-7	methyl myristate	1	2
	C ₁₅ H ₃₀ O ₂	10233-13-3	isopropyl laurate	1	2
	C ₁₄ H ₂₈ O ₂	544-63-8	Myristic acid	1	2
	C ₁₅ H ₂₈ O ₂	106-02-5	pentadecan-15-olide	1	2
	C ₇ H ₅ NO	103-71-9	Phenylisocyanate	1	2
	C ₁₅ H ₁₁ ClO ₃	2536-31-4	Chlorflurenol-methyl (ester)	2	2
	C ₁₆ H ₁₀ ClN ₃ O ₃	2814-77-9	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	2	2
	C ₁₆ H ₃₂ O ₂	2306-88-9	octyl octanoate	2	2
	C ₁₆ H ₃₂ O ₂	57-10-3	Hexadecanoic acid	2	2
		1799-84-4	4:2 FTMAC	5	2
		68259-15-4	MeFHxSA	2	2
		80-09-1	bisphenol S	3	1
		620-92-8	4,4'-BPF	4	1
		13595-25-0	bisphenol M	5	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		137862-53-4	Valsartan	3	2
		4065-45-6	benzophenone-4 (sulisobenzene)	5	2
		27503-81-7	PBS (Phenylbenzimidazole sulfonic acid)	7	2

Table 16: Effluent Greenland

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
52627,52	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	6	2
26654,10	C8H10N4O2	58-08-2	Caffeine	7	3
14634,51	C8H7N	120-72-9	Indole	1	2
11227,99	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	7	2
6470,04	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
6194,59	C10H20O	15356-70-4	DL-Menthol	3	2
5603,52	C24H38O4	6422-86-2	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	1	3
5546,29	C8H10O	60-12-8	Phenylethyl Alcohol	2	3
4470,41	C10H22O	78-69-3	3-Octanol, 3,7-dimethyl-	3	2
3840,42	C16H34O3	3055-93-4	Diethylene glycol monododecyl ether	1	2
2506,84	C18H26O	1222-05-5	Galaxolide	6	2
2073,93	C11H20O2	104-67-6	2(3H)-Furanone, 5-heptyldihydro-	1	2
1955,10	C14H26O2	544-64-9	Myristoleic acid	1	2
1897,06	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
1693,75	C9H9N	83-34-1	1H-Indole, 3-methyl-	2	2
1562,43	C20H32O2	-	Benzoic acid, tridecyl ester	7	3
1415,24	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	5	2
1271,36	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	7	3
1239,19	C10H14O	39852-87-4	Tricyclo[5.2.1.0(2,6)]dec-3-en-10-ol	2	3
1161,01	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	4	2
1148,82	C8H5NO2	91-56-5	1H-Indole-2,3-dione	1	3
1093,29	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
957,14	C10H22O3	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	5	3
878,50	C8H10O	123-07-9	Phenol, 4-ethyl-	1	2
782,64	C14H11N	611-64-3	Acridine, 9-methyl-	5	2
744,70	C12H22O2	1900-69-2	Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate, trans-	2	2
695,40	C17H25NO4	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	1	2
677,46	C22H36O2	-	Benzoic acid, pentadecyl ester	6	3
632,46	C18H26O3	83834-59-7	2-Ethylhexyl trans-4-methoxycinnamate	1	2
621,12	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	4	2
502,22	C18H30	2719-62-2	Benzene, (1-pentylheptyl)-	1	2
439,92	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	1	2
435,63	C8H9NO2	134-20-3	Methyl anthranilate	1	2
400,28	C13H10O	119-61-9	Benzophenone	7	2
356,47	C8H7NO	2380-94-1	1H-Indol-4-ol	2	3
341,85	C8H6O2	1074-12-0	Phenylglyoxal	6	2
335,67	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
299,18	C13H28O4	55934-93-5	Propanol, [(butoxymethylethoxy)methylethoxy]-	1	2
253,14	C17H28	4537-15-9	Benzene, (1-butylheptyl)-	1	2
217,46	C9H7NO	487-89-8	1H-Indole-3-carboxaldehyde	1	2
189,50	C7H8O	108-39-4	Phenol, 3-methyl-	3	2
186,90	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
168,37	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	1	2
148,74	C14H8N2S2	4271-09-4	2,2'-Bibenzothiazole	1	3
144,21	C10H14O	99-49-0	Carvone	5	2
124,51	C11H13ClO	-	3-Buten-1-ol, 4-chloro-2-methyl-1-phenyl-	3	2
94,78	C10H15NO2S	3622-84-2	Benzenesulfonamide, N-butyl-	3	2
85,86	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	1	2
79,19	C7H5NOS	934-34-9	2(3H)-Benzothiazolone	2	3
67,22	C9H6O2	91-64-5	Coumarin	3	2
46,62	C8H14O4	627-93-0	Hexanedioic acid, dimethyl ester	5	3
41,63	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
12,54	C17H34O	55019-46-0	Hexadecanal, 2-methyl-	1	2
	C20H25ClN2O5	-	Amlodipine	6	2
	C38H52N6O7	-	Atazanavir	5	2
	C14H22N2O3	-	Atenolol	7	2
	C8H10N4O2	-	Caffeine	7	2
	C15H12N2O	-	Carbamazepine	7	2
	C15H14N2O3	-	Carbamazepine, 10, 11-dihydroxy	7	2
	C15H14N2O2	-	Carbamazepine, 10-hydroxy	7	2
	C21H25ClN2O3	-	Cetirizine	7	2
	C17H18FN3O3	-	Ciprofloxacin	7	2
	C19H19FN2O	-	Citalopram, Desmethyl	4	2

Continued					
Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₂₀ H ₂₁ FN ₂ O		Citalopram/Escitalopram	7	2
	C ₁₈ H ₁₉ ClN ₄		Clozapine	7	2
	C ₁₀ H ₁₂ N ₂ O		Cotinine	7	2
	C ₃₂ H ₃₉ NO ₄		Fexofenadine	7	2
	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄		Ketoconazole	7	2
	C ₉ H ₇ Cl ₂ N ₅		Lamotrigine	7	2
	C ₂₂ H ₂₃ ClN ₆ O		Losartan	7	2
	C ₁₅ H ₂₅ NO ₃		Metoprolol	7	2
	C ₁₇ H ₁₉ N ₃		Mirtazapine	7	2
	C ₁₀ H ₁₄ N ₂		Nicotine	7	2
	C ₁₆ H ₂₁ NO ₂		Propranolol	7	2
	C ₂₁ H ₂₅ N ₃ O ₂ S		Quetiapine	7	2
	C ₂₀ H ₂₄ N ₂ O ₂		Quinine	7	2
	C ₁₁ H ₁₁ N ₃ O ₂ S		Sulfapyridine	7	2
	C ₁₄ H ₂₁ N ₃ O ₂ S		Sumatriptan	7	2
	C ₁₆ H ₂₅ NO ₂		Tramadol	7	2
	C ₁₄ H ₁₈ N ₄ O ₃		Trimethoprim	7	2
	C ₁₇ H ₂₇ NO ₂		Venlafaxine	7	2
	C ₁₆ H ₂₅ NO ₂		Venlafaxine,-O-demethyl-	8	2
	C ₉ H ₁₁ NO ₂	94-09-7	BENZOCAINE	10	2
	C ₈ H ₉ NO ₂	103-90-2	paracetamol	11	2
	C ₇ H ₇ NO ₅ S	121-03-9	4-nitrotoluene-2-sulphonic acid	2	2
	C ₁₂ H ₂₄ O ₂	143-07-7	Neo-Fat 12-43	1	2
	C ₁₈ H ₃₆ O ₃	106-14-9	12-hydroxystearic acid	1	2
		1799-84-4	4:2 FTMAC	5	2
		106-44-5	p-cresol	1	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		3233-32-7	4-acetoxyphenol	1	2
		103-90-2	paracetamol	5	2

Table 17: Effluent Faroe Islands

Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
6515,32	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	6	2
2910,65	C10H20O	89-78-1	DL-Menthol	3	2
2366,64	C8H10N4O2	58-08-2	Caffeine	7	3
1909,34	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	7	3
1782,73	C9H12O	617-94-7	Benzenemethanol, à,à-dimethyl-	1	2
1472,49	C9H9N	83-34-1	1H-Indole, 3-methyl-	2	2
1179,06	C10H22O	78-69-3	3-Octanol, 3,7-dimethyl-	3	2
1019,71	C14H31N	112-18-5	1-Dodecanamine, N,N-dimethyl-	1	3
343,58	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
263,73	C10H14O	99-49-0	Carvone	5	2
258,63	C8H6O2	1074-12-0	Phenylglyoxal	6	2
231,30	C18H26O	1222-05-5	Galaxolide	6	2
194,73	C10H22O3	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	5	3
183,48	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
161,29	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
104,03	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	7	2
78,39	C12H22O2	1900-69-2	Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate, trans-	2	2
70,46	C13H10O	119-61-9	Benzophenone	7	2
60,12	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	7	3
56,99	C20H32O2	-	Benzoic acid, tridecyl ester	7	3
42,46	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	5	2
37,64	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	5	2
34,13	C22H36O2	-	Benzoic acid, pentadecyl ester	6	3
23,35	C9H6O2	91-64-5	Coumarin	3	2
	C20H23N		Amitriptyline	6	2
	C20H25ClN2O5		Amlodipine	6	2
	C14H22N2O3		Atenolol	7	2
	C38H72N2O12		Azithromycin	6	2
	C8H10N4O2		Caffeine	7	2
	C15H12N2O		Carbamazepine	7	2
	C15H14N2O3		Carbamazepine, 10, 11-dihydroxy	7	2
	C15H14N2O2		Carbamazepine, 10-hydroxy	7	2
	C21H25ClN2O3		Cetirizine	7	2
	C17H18FN3O3		Ciprofloxacin	7	2
	C20H21FN2O		Citalopram/Escitalopram	7	2
	C38H69NO13		Clarithromycin	6	2
	C18H19ClN4		Clozapine	7	2
	C17H17ClN4		Clozapine, Desmethyl	6	2
	C18H21NO3		Codeine	6	2
	C10H12N2O		Cotinine	7	2
	C22H26N2O4S		Diltiazem	6	2
	C24H40N8O4		Dipyridamol	4	2
	C32H39NO4		Fexofenadine	7	2
	C18H21NO3		Hydrocodone	6	2
	C26H28Cl2N4O4		Ketoconazole	7	2
	C9H7Cl2N5		Lamotrigine	7	2
	C22H23ClN6O		Losartan	7	2
	C20H23N		Maprotiline	6	2
	C14H22ClN3O2		Metoclopramide	6	2
	C15H25NO3		Metoprolol	7	2
	C17H19N3		Mirtazapine	7	2
	C10H14N2		Nicotine	7	2
	C15H11ClN2O2		Oxazepam	6	2
	C16H21NO2		Propranolol	7	2
	C21H25N3O2S		Quetiapine	7	2
	C20H24N2O2		Quinine	7	2
	C12H20N2O3S		Sotalol	6	2
	C11H11N3O2S		Sulfapyridine	7	2
	C14H21N3O2S		Sumatriptan	7	2
	C16H25NO2		Tramadol	7	2
	C14H18N4O3		Trimethoprim	7	2
	C17H27NO2		Venlafaxine	7	2

Continued					
Quant (ng/L)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₁₆ H ₂₅ NO ₂		Venlafaxine, -O-demethyl-	7	2
	C ₇ H ₇ NO ₅ S	121-03-9	4-nitrotoluene-2-sulphonic acid	2	2
	C ₉ H ₁₁ NO ₃	69-96-5	beta-hydroxyphenylalanine	1	2
	C ₁₇ H ₃₄ O ₂	6309-51-9	isopentyl laurate	3	2
	C ₁₇ H ₃₄ O ₂	110-27-0	Wickenol 101	3	2
	C ₁₇ H ₃₄ O ₂	112-39-0	methyl palmitate	2	2
	C ₈ H ₅ NO ₂	85-41-6	1H-Isoindole-1,3(2H)-dione	2	2
	C ₇ H ₉ NO ₂	30652-11-0	Deferiprone	2	2
	C ₉ H ₁₁ NO ₂	938-73-8	ethenzamide	1	2
	C ₁₆ H ₃₂ O ₂	2306-88-9	octyl octanoate	2	2
	C ₁₆ H ₃₂ O ₂	57-10-3	Hexadecanoic acid	2	2
	C ₈ H ₉ NO ₂	103-90-2	paracetamol	5	2
	C ₉ H ₁₉ NO ₄	16485-10-2	panthenol , DL-form	2	2
	C ₁₁ H ₁₂ N ₂ O ₂	73-22-3	Tryptophan	1	2
		1799-84-4	4:2 FTMAC	5	2
		80-09-1	bisphenol S	3	1
		13595-25-0	bisphenol M	5	1
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		27503-81-7	PBS (Phenylbenzimidazole sulfonic acid)	7	2
		103-90-2	paracetamol	5	2

Table 18: Sediment Finland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
272,77	C ₂₃ H ₃₆ O ₄	-	Phthalic acid, hept-3-yl octyl ester	6	2
143,64	C ₁₆ H ₁₀	206-44-0	Fluoranthene	6	2
136,61	C ₁₆ H ₁₀	129-00-0	Pyrene	6	2
99,31	C ₂₀ H ₁₂	205-99-2	Benz[b]fluoranthene	1	2
82,86	C ₁₄ H ₁₀	85-01-8	Phenanthrene	6	2
63,91	C ₁₈ H ₁₂	217-59-4	Triphenylene	6	2
58,31	C ₃₀ H ₄₈ O	-	4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	2	3
45,63	C ₂₀ H ₁₂	198-55-0	Perylene	5	2
44,49	C ₃₀ H ₄₈ O	1617-70-5	Lupenone	2	3
43,28	C ₁₈ H ₁₂	56-55-3	Benz[a]anthracene	6	2
41,80	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
40,34	C ₇ H ₅ NS	95-16-9	Benzothiazole	6	2
40,23	C ₂₀ H ₁₂	192-97-2	Benzo[e]pyrene	5	2
38,80	C ₁₄ H ₁₄ O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
36,83	C ₉ H ₁₂ O ₂	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
36,06	C ₁₃ H ₁₆ O	55591-10-1	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-	4	3
34,55	C ₂₂ H ₁₂	193-39-5	Indeno[1,2,3-cd]pyrene	4	2
33,75	C ₃₀ H ₅₀	1615-91-4	Diploptene	4	3
30,73	C ₂₀ H ₁₂	50-32-8	Benzo[a]pyrene	5	2
28,93	C ₁₁ H ₁₆ O ₂	15356-74-8	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	5	2
24,53	C ₁₀ H ₈	91-20-3	Naphthalene	4	2
21,25	C ₁₈ H ₁₈	66552-97-4	2-Isopropyl-10-methylphenanthrene	5	3
21,01	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
20,26	C ₁₇ H ₁₂	199-94-0	7H-Benzo[de]anthracene	4	3
19,27	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
19,11	C ₁₂ H ₆ Cl ₄	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
17,04	C ₁₆ H ₁₆	7694-30-6	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	5	2
16,61	C ₁₉ H ₁₄	82979-72-4	8,9-Dihydro-7H-cyclopenta[a]pyrene	5	3
16,36	C ₁₄ H ₁₀	120-12-7	Anthracene	6	2
14,98	C ₁₅ H ₁₂	27410-55-5	8,9-Dihydrocyclopenta[def]phenanthrene	5	3
13,31	C ₁₁ H ₁₄ O ₄	-	1-Methyl-1,3-cyclohexadiene-5,6-diol diacetate	3	3
12,83	C ₁₆ H ₁₀ O	205-39-0	Benzo(b)naphtho[1,2-d]furan	5	3
12,71	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
12,53	C ₇ H ₇ NO ₂	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
12,42	C ₁₀ H ₁₆	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	4	3
11,17	C ₅ H ₉ NO ₂	4394-85-8	N-Formylmorpholine	2	2
11,15	C ₂₂ H ₁₂	193-43-1	Indeno[1,2,3-cd]fluoranthene	4	2
11,10	C ₂₂ H ₃₄ O ₄	-	Phthalic acid, nonyl 2-pentyl ester	2	2
10,70	C ₁₂ H ₈ O	132-64-9	Dibenzofuran	5	2
9,94	C ₁₅ H ₁₀	83469-43-6	6H-Cyclobuta[jk]phenanthrene	5	2
9,89	C ₁₈ H ₃₀	2719-62-2	Benzene, (1-pentylheptyl)-	4	2
9,87	C ₁₆ H ₁₀ S	205-43-6	Benzo[b]naphtho[1,2-d]thiophene	5	2
9,31	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	5	2
9,22	C ₁₂ H ₁₂	-	Naphthalene, dimethyl-	10	3
8,78	C ₁₃ H ₁₄	829-26-5	Naphthalene, 2,3,6-trimethyl-	4	2
8,73	C ₁₃ H ₁₀	86-73-7	Fluorene	4	2
8,64	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
8,56	C ₁₈ H ₂₂	6566-19-4	10,18-Bisnorabieta-5,7,9(10),11,13-pentaene	3	3
8,54	C ₁₅ H ₂₈	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	3	3
8,10	C ₁₃ H ₈ O	548-39-0	1H-Phenalen-1-one	4	2
7,74	C ₈ H ₇ NS ₂	615-22-5	Benzothiazole, 2-(methylthio)-	2	2
7,53	C ₈ H ₈ O ₃	121-33-5	Vanillin	2	2
7,47	C ₉ H ₁₀ O ₂	101-41-7	Phenylacetic acid, methyl ester	2	2
7,38	C ₁₂ H ₆ Cl ₄	-	1,1'-Biphenyl, 2,2',5,5'-tetramethyl- (isomer)	3	3
7,34	C ₁₅ H ₁₂	832-71-3	Phenanthrene, 3-methyl-	4	2
7,16	C ₁₇ H ₂₈	4537-15-9	Benzene, (1-butylheptyl)-	3	2
6,99	C ₁₆ H ₁₂	6232-48-0	Acephenanthrylene, 4,5-dihydro-	5	2
6,87	C ₁₁ H ₁₀	91-57-6	Naphthalene, 2-methyl-	6	2
6,81	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
5,73	C ₁₇ H ₁₆	3674-73-5	Phenanthrene, 2,3,5-trimethyl-	4	2
5,56	C ₁₁ H ₁₈ O ₄	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	3	2
5,49	C ₁₇ H ₁₂	243-17-4	11H-Benzo[b]fluorene	5	2

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
5,02	C12H12	-	Naphthalene, dimethyl-	10	3
4,98	C16H14	3674-69-9	Phenanthrene, 4,5-dimethyl-	5	2
4,97	C17H12	-	7H-Benzo[c]fluorene (isomer)	13	3
4,94	C15H8O	5737-13-3	Cyclopenta(def)phenanthrenone	4	2
4,89	C16H11N	-	11H-Benzo[a]carbazole (isomer)	7	3
4,76	C9H14O6	102-76-1	Triacetin	3	2
4,75	C21H36	641-85-0	Allopregnane	3	3
4,72	C18H10	203-12-3	Benzo[ghi]fluoranthene	3	2
4,67	C16H10O	200-23-7	Benzo[kl]xanthene	4	3
4,45	C20H12	205-82-3	Benzo[j]fluoranthene	4	2
3,92	C16H14	1576-67-6	Phenanthrene, 3,6-dimethyl-	5	2
3,89	C14H8O2	84-65-1	9,10-Anthracenedione	5	2
3,79	C17H10O	82-05-3	7H-Benz[de]anthracene-7-one	4	2
3,75	C11H10	90-12-0	Naphthalene, 1-methyl-	6	2
3,70	C9H7NO	487-89-8	1H-Indole-3-carboxaldehyde	3	2
3,55	C16H10O	243-42-5	Benzo[b]naphtho[2,3-d]furan	4	3
3,31	C21H14	63104-32-5	10-Methylbenzo(a)pyrene	4	3
3,26	C16H10S	227-86-1	Anthra(1,2-b)thiophene	3	3
3,22	C18H10O	191-37-7	Naphtho[2,1,8,7-klmn]xanthene	4	3
3,18	C18H12	195-19-7	Benzo[c]phenanthrene	5	2
3,15	C13H10O	92-83-1	9H-Xanthene	5	2
2,95	C19H12	50861-05-7	9H-Cyclopenta[a]pyrene	5	2
2,91	C18H14S	24964-16-7	Benzo[b]naphtho[2,3-d]thiophene, 7,8-dimethyl-	3	3
2,89	C10H12O	487-68-3	Benzaldehyde, 2,4,6-trimethyl-	3	3
2,80	C20H16	35187-19-0	4,12-Dimethylbenz[a]anthracene	4	3
2,80	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	3	2
2,77	C11H20	2958-76-1	Naphthalene, decahydro-2-methyl-	2	2
2,61	C15H22	483-77-2	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	3	2
2,53	C16H11N	243-28-7	Benzo(b)carbazole	2	2
2,50	C21H14	239-85-0	13H-Dibenzo[a,h]fluorene	5	3
2,46	C15H12	832-64-4	Phenanthrene, 4-methyl-	4	2
2,39	C21H14	241-28-1	8H-Indeno[2,1-b]phenanthrene	4	3
2,35	C10H14	488-23-3	Benzene, 1,2,3,4-tetramethyl-	3	2
2,33	C16H10S	239-35-0	Benzo[b]naphtho[2,1-d]thiophene	3	2
2,29	C17H12S	-	2-Methylbenzo[b]naphtho[2,1-d]thiophene	3	3
2,24	C6H11NO2	1696-20-4	Morpholine, 4-acetyl-	1	3
2,09	C14H12S	1136-85-2	3,7-Dimethyldibenzothiophene	3	2
1,94	C20H14	612-78-2	2,2'-Binaphthalene	3	3
1,78	C20H32O2	-	Benzoic acid, tridecyl ester	4	3
1,74	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
1,72	C14H14	613-33-2	4,4'-Dimethylbiphenyl	3	2
1,70	C12H12O5	5062-30-6	Phenacylidene diacetate	2	2
1,63	C16H11N	-	11H-Benzo[a]carbazole (isomer)	7	3
1,55	C22H36O2	-	Benzoic acid, pentadecyl ester	5	3
1,54	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	5	3
1,52	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	3	2
1,07	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	3	2
0,89	C13H12	643-93-6	1,1'-Biphenyl, 3-methyl-	3	2
	C13H16O5	99469-99-5	ethyl 2-ethoxy-4-carboxymethylbenzoate	2	2
		17202-41-4	PFNS	1	2
	C12HF23O2	307-55-1	PFDOA	1	2
		92612-52-7	PFHxA	4	2
		39108-34-4	8:2 FTS	1	2
		355-46-4	PFHxS	1	2
	C9H6F12O	78971-81-0		1	2
		40143-77-9	C6/C6-PFPIA	1	2
	C18H11F19O2	94159-92-9		1	2
		1478-61-1	hexafluoroBPA (bisfenol AF)	1	1
		843-55-0	bisfenol Z	3	1
		13595-25-0	bisphenol M	3	1
		5835-26-7	isopimaric acid	4	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2

Table 19: Sediment Sweden

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
1594,44	C20H12	205-99-2	Benzo[b]fluoranthene	4	2
1108,95	C16H10	206-44-0	Fluoranthene	6	2
811,12	C22H12	193-39-5	Indeno[1,2,3-cd]pyrene	4	2
755,77	C20H12	192-97-2	Benzo[e]pyrene	5	2
711,73	C20H12	50-32-8	Benzo[a]pyrene	5	2
623,82	C18H12	217-59-4	Triphenylene	6	2
603,09	C30H50	1615-91-4	Diploptene	4	3
471,01	C18H12	56-55-3	Benz[a]anthracene	6	2
391,03	C30H48O	1617-70-5	Lupenone	2	3
389,23	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
363,59	C12H12	-	Naphthalene, dimethyl-	10	3
266,21	C18H18	66552-97-4	2-Isopropyl-10-methylphenanthrene	5	3
244,63	C20H12	198-55-0	Perylene	5	2
236,31	C11H16O2	15356-74-8	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	5	2
227,71	C18H22	6566-19-4	10,18-Bisnorabieta-5,7,9(10),11,13-pentaene	3	3
226,99	C13H16O	55591-10-1	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-	4	3
194,71	C19H14	82979-72-4	8,9-Dihydro-7H-cyclopenta[a]pyrene	5	3
179,94	C17H12	199-94-0	7H-Benzo[de]anthracene	4	3
179,52	C21H14	63104-32-5	10-Methylbenzo(a)pyrene	4	3
175,34	C14H10	120-12-7	Anthracene	6	2
175,25	C20H12	205-82-3	Benzo[j]fluoranthene	4	2
153,13	C22H34O4	-	Phthalic acid, nonyl 2-pentyl ester	2	2
127,93	C17H12	-	7H-Benzo[c]fluorene isomer	2	3
126,15	C16H10S	205-43-6	Benzo[b]naphtho[1,2-d]thiophene	5	2
116,02	C13H20O	79-77-6	trans-á-Ionone	1	2
115,30	C21H14	241-28-1	8H-Indeno[2,1-b]phenanthrene	4	3
110,32	C16H10O	205-39-0	Benzo(b)naphtho(1,2-d)furan	5	3
100,41	C20H16	35187-19-0	4,12-Dimethylbenz[a]anthracene	4	3
86,84	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
78,80	C17H16	3674-73-5	Phenanthrene, 2,3,5-trimethyl-	4	2
77,44	C21H14	239-85-0	13H-Dibenzo[a,h]fluorene	5	3
75,94	C15H12	832-69-9	Phenanthrene, 1-methyl-	3	2
68,22	C18H12	195-19-7	Benzo[c]phenanthrene	5	2
65,28	C21H36	641-85-0	Allopregnane	3	3
62,75	C12H8O	132-64-9	Dibenzofuran	5	2
61,98	C15H10	83469-43-6	6H-Cyclobuta[jk]phenanthrene	5	2
58,83	C12H12	-	Naphthalene, dimethyl-	10	3
58,62	C16H14	3674-69-9	Phenanthrene, 4,5-dimethyl-	5	2
57,53	C7H7NO2	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
57,24	C16H10O	200-23-7	Benzo[k]xanthene	4	3
56,86	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
55,56	C17H12	-	7H-Benzo[c]fluorene (isomer)	13	3
55,39	C18H10O	191-37-7	Naphtho[2,1,8,7-klmn]xanthene	4	3
55,35	C13H10	86-73-7	Fluorene	4	2
53,15	C18H10	203-12-3	Benzo[ghi]fluoranthene	3	2
52,75	C16H12	6232-48-0	Acephenanthrylene, 4,5-dihydro-	5	2
46,53	C16H14	1576-67-6	Phenanthrene, 3,6-dimethyl-	5	2
45,40	C16H11N	-	11H-Benzo[a]carbazole (isomer)	7	3
44,67	C15H12	832-71-3	Phenanthrene, 3-methyl-	4	2
44,44	C16H16	7694-30-6	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	5	2
37,75	C11H10	91-57-6	Naphthalene, 2-methyl-	6	2
36,84	C13H10O	3218-36-8	[1,1'-Biphenyl]-4-carboxaldehyde	4	2
36,79	C17H12	243-17-4	11H-Benzo[b]fluorene	5	2
36,77	C17H12S	-	2-Methylbenzo[b]naphtho[2,1-d]thiophene	3	3
34,41	C14H12S	1136-85-2	3,7-Dimethyldibenzothiophene	3	2
34,27	C16H10S	227-86-1	Anthra(1,2-b)thiophene	3	3
32,43	C18H14S	24964-12-3	Benzo[b]naphtho[2,3-d]thiophene, 7,8-dimethyl-	3	3
32,04	C17H12	-	7H-Benzo[c]fluorene (isomer)	13	3
30,67	C16H11N	243-28-7	Benzo(b)carbazole	2	2
29,34	C16H10O	243-42-5	Benzo[b]naphtho[2,3-d]furan	4	3
29,09	C17H11N	225-51-4	Benz[c]acridine	2	3
25,68	C17H10O	82-05-3	7H-Benz[de]anthracen-7-one	4	2
25,58	C16H11N	-	11H-Benzo[a]carbazole (isomer)	7	3

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
24,40	C15H12	832-64-4	Phenanthrene, 4-methyl-	4	2
21,60	C20H14	612-78-2	2,2'-Binaphthalene	3	3
20,47	C16H10S	239-35-0	Benzo[b]naphtho[2,1-d]thiophene	3	2
18,21	C15H8O	5737-13-3	Cyclopenta(def)phenanthrenone	4	2
18,15	C14H8O2	84-65-1	9,10-Anthracenedione	5	2
17,49	C19H12	50861-05-7	9H-Cyclopenta[a]pyrene	5	2
16,29	C13H10O	92-83-1	9H-Xanthene	5	2
15,39	C9H7NO	487-89-8	1H-Indole-3-carboxaldehyde	3	2
15,06	C13H8O	548-39-0	1H-Phenalen-1-one	4	2
12,07	C9H14O6	102-76-1	Triacetin	3	2
9,18	C11H20	-	trans-Decalin, 2-methyl-	1	2
8,97	C8H8O3	121-33-5	Vanillin	2	2
8,84	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	2	2
8,84	C12H22O2	1900-69-2	Cyclohexanol, 4-(1,1-dimethylethyl)-, acetate, trans-	1	2
8,69	C24H38O4	6422-86-2	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2	3
7,88	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	4	3
7,79	C12H22	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	1	3
6,97	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester:2	1	2
6,91	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	3	2
6,9	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
6,86	C6H5Cl2N	608-27-5	Benzenamine, 2,3-dichloro-	1	2
6,74	C15H28	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	3	3
6,66	C10H14	527-53-7	Benzene, 1,2,3,5-tetramethyl-	2	2
6,32	C9H10O2	101-41-7	Phenylacetic acid, methyl ester	2	2
6,19	C18H30	2719-62-2	Benzene, (1-pentylheptyl)-	4	2
6,11	C17H28	4537-15-9	Benzene, (1-butylheptyl)-	3	2
6,04	C11H20O2	104-67-6	2(3H)-Furanone, 5-heptyldihydro-	1	2
5,93	C12H22	66660-41-1	2-Ethyldecahydronaphthalene, (Z,E)-	1	2
5,9	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
5,76	C13H16	30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	1	2
5,58	C18H28O2	6316-30-9	Benzoic acid, undecyl ester	5	3
5,53	C22H36O2	-	Benzoic acid, pentadecyl ester	5	3
5,47	C6H4Cl3N	634-91-3	Benzenamine, 3,4,5-trichloro-	1	2
5,47	C10H12O	487-68-3	Benzaldehyde, 2,4,6-trimethyl-	3	3
5,15	C9H8O	83-33-0	1H-Inden-1-one, 2,3-dihydro-	1	2
4,91	C11H10	90-12-0	Naphthalene, 1-methyl-	6	2
4,84	C7H5NS	95-16-9	Benzothiazole	6	2
4,83	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	3	2
4,76	C14H14	613-33-2	4,4'-Dimethylbiphenyl	3	2
4,72	C9H9N	83-34-1	1H-Indole, 3-methyl-	1	2
4,6	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
4,54	C8H7N	120-72-9	Indole	2	2
4,48	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	3	2
4,41	C11H14O4	-	1-Methyl-1,3-cyclohexadiene-5,6-diol diacetate	3	3
4,27	C15H22	483-77-2	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	3	2
4,27	C13H18	30316-36-0	Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	1	2
4,14	C10H8	91-20-3	Naphthalene	4	2
4,1	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	3	2
3,87	C13H10O	119-61-9	Benzophenone	7	2
3,85	C7H4ClNO	2909-38-8	Benzene, 1-chloro-3-isocyanato-	1	3
3,77	C18H26O	1222-05-5	Galaxolide	2	2
3,73	C13H12	643-93-6	1,1'-Biphenyl, 3-methyl-	3	2
3,54	C10H14	488-23-3	Benzene, 1,2,3,4-tetramethyl-	3	2
3,2	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
2,91	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl- (isomer)	3	3
2,89	C15H12	27410-55-5	8,9-Dihydrocyclopenta[def]phenanthrene	5	3
2,86	C8H7NO	2380-94-1	1H-Indol-4-ol	2	3
2,69	C30H48O	-	4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	2	3
2,44	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	3	2
2,18	C13H14	829-26-5	Naphthalene, 2,3,6-trimethyl-	4	2
1,24	C22H12	193-43-1	Indeno[1,2,3-cd]fluoranthene	4	2
1,23	C16H10	129-00-0	Pyrene	6	2
1,08	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	6	2

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
-0,58	C ₁₂ H ₅ Cl ₅	32598-14-4	1,1'-Biphenyl, 2,3,3',4,4'-pentachloro-	2	2
-0,96	C ₁₄ H ₁₀	85-01-8	Phenanthrene	6	2
		4247-02-3	isobutyl 4-hydroxybenzoate	1	2
		99469-99-5	ethyl 2-ethoxy-4-carboxymethylbenzoate	2	2
		92612-52-7	PFHxA	4	2
		106-44-5	p-cresol	1	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2

Table 20: Sediment Denmark

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
265,66	C16H10	206-44-0	Fluoranthene	6	2
204,98	C16H10	129-00-0	Pyrene	6	2
174,27	C20H12	207-08-9	Benzo[k]fluoranthene	1	2
166,08	C20H12	205-99-2	Benzo[b]fluoranthene	4	2
136,36	C22H12	193-39-5	Indeno[1,2,3-cd]pyrene	4	2
132,12	C30H50	1615-91-4	Diploptene	4	3
111,81	C20H12	192-97-2	Benzo[e]pyrene	5	2
106,32	C20H12	50-32-8	Benzo[a]pyrene	5	2
92,74	C18H12	217-59-4	Triphenylene	6	2
87,77	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
85,20	C22H12	193-43-1	Indeno[1,2,3-cd]fluoranthene	4	2
84,02	C11H16O2	15356-74-8	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	5	2
82,77	C18H12	56-55-3	Benz[a]anthracene	6	2
63,89	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	6	2
62,67	C7H9NO2	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
40,26	C14H10	85-01-8	Phenanthrene	6	2
36,01	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	3	2
36,01	C13H20O	79-77-6	trans-beta-Ionone	1	2
29,89	C13H16O	55591-10-1	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-	4	3
27,69	C7H5NS	95-16-9	Benzo[thiazole]	6	2
27,31	C20H12	205-82-3	Benzo[j]fluoranthene	4	2
25,69	C13H10O	119-61-9	Benzophenone	7	2
25,24	C16H10O	205-39-0	Benzo(b)naphtho(1,2-d)furan	5	3
24,98	C17H12	199-94-0	7H-Benzo[de]anthracene	4	3
21,48	C16H16	7694-30-6	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	5	2
19,89	C14H10	120-12-7	Anthracene	6	2
16,36	C17H12	-	7H-Benzo[c]fluorene isomer	2	3
16,34	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
14,63	C11H14O4	-	1-Methyl-1,3-cyclohexadiene-5,6-diol diacetate	3	3
14,56	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	2	2
14,48	C20H12	198-55-0	Perylene	5	2
13,81	C19H14	82979-72-4	8,9-Dihydro-7H-cyclopenta[a]pyrene	5	3
13,66	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
13,46	C16H10S	205-43-6	Benzo[b]naphtho[1,2-d]thiophene	5	2
12,91	C15H12	27410-55-5	8,9-Dihydrocyclopenta[def]phenanthrene	5	3
12,78	C17H12	-	7H-Benzo[c]fluorene (isomer)	13	(isomer)
11,80	C15H10	83469-43-6	6H-Cyclobuta[jk]phenanthrene	5	2
11,15	C16H12	6232-48-0	Acephenanthrylene, 4,5-dihydro-	5	2
10,74	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
9,17	C16H10O	200-23-7	Benzo[k]xanthene	4	3
8,78	C10H8	91-20-3	Naphthalene	4	2
8,40	C18H12	195-19-7	Benzo[c]phenanthrene	5	2
8,11	C17H10O	82-05-3	7H-Benz[de]anthracen-7-one	4	2
7,94	C21H14	239-85-0	13H-Dibenzo[a,h]fluorene	5	3
7,50	C16H10O	243-42-5	Benzo[b]naphtho[2,3-d]furan	4	3
7,41	C15H12	832-69-9	Phenanthrene, 1-methyl-	3	2
7,36	C17H12	243-17-4	11H-Benzo[b]fluorene	5	2
7,35	C15H12	832-71-3	Phenanthrene, 3-methyl-	4	2
7,30	C21H14	241-28-1	8H-Indeno[2,1-b]phenanthrene	4	3
6,83	C12H8O	132-64-9	Dibenzofuran	5	2
6,27	C17H11N	225-51-4	Benz[c]acridine	2	3
6,02	C17H12	-	7H-Benzo[c]fluorene (isomer)	13	3
5,75	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	5	2
5,57	C16H14	3674-69-9	Phenanthrene, 4,5-dimethyl-	5	2
5,50	C16H20	24157-81-1	2,6-Diisopropyl-naphthalene	3	2
5,44	C19H12	50861-05-7	9H-Cyclopenta[a]pyrene	5	2
5,24	C7H7NO2	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
4,74	C21H14	63104-32-5	10-Methylbenzo(a)pyrene	4	3
4,62	C11H10	91-57-6	Naphthalene, 2-methyl-	6	2
4,43	C12H12	-	Naphthalene, dimethyl-	10	3
4,19	C16H14	1576-67-6	Phenanthrene, 3,6-dimethyl-	5	2
3,78	C18H18	66552-97-4	2-Isopropyl-10-methylphenanthrene	5	3

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3,78	C ₁₄ H ₈ O ₂	84-65-1	9,10-Anthracenedione	5	2
3,67	C ₁₃ H ₁₀ O	3218-36-8	[1,1'-Biphenyl]-4-carboxaldehyde	4	2
3,50	C ₁₀ H ₁₂ O	487-68-3	Benzaldehyde, 2,4,6-trimethyl-	3	3
3,32	C ₁₂ H ₁₂	-	Naphthalene, dimethyl-	10	3
3,11	C ₁₁ H ₁₀	90-12-0	Naphthalene, 1-methyl-	6	2
2,77	C ₁₃ H ₁₀ O	92-83-1	9H-Xanthene	5	2
2,30	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
	C ₁₃ H ₈ F ₂₁ O ₅ P	94158-70-0		1	2
		843-55-0	bisfenol Z	3	1
		13595-25-0	bisphenol M	3	1
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2

Table 21: Sediment Iceland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
66,60	C ₂₃ H ₃₆ O ₄	-	Phthalic acid, hept-3-yl octyl ester	6	2
38,76	C ₁₅ H ₂₄	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
37,70	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
37,05	C ₁₄ H ₁₄ O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
15,94	C ₇ H ₅ NS	95-16-9	Benothiazole	6	2
15,62	C ₁₂ H ₆ Cl ₄	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
12,05	C ₉ H ₁₂ O ₂	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
9,94	C ₁₈ H ₁₂	217-59-4	Triphenylene	6	2
8,82	C ₆ H ₅ BrO	591-20-8	Phenol, 3-bromo-	2	2
8,05	C ₈ H ₇ N	120-72-9	Indole	2	2
7,89	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	4	3
7,65	C ₁₄ H ₁₀	120-12-7	Anthracene	6	2
6,58	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
6,37	C ₁₄ H ₁₀	85-01-8	Phenanthrene	6	2
6,35	C ₁₆ H ₁₀	129-00-0	Pyrene	6	2
6,34	C ₂₂ H ₃₆ O ₂	-	Benzoic acid, pentadecyl ester	5	3
6,33	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	5	3
6,12	C ₁₆ H ₁₀	206-44-0	Fluoranthene	6	2
6,09	C ₈ H ₇ NO	2380-94-1	1H-Indol-4-ol	2	3
5,99	C ₅ H ₉ NO ₂	4394-85-8	N-Formylmorpholine	2	2
5,08	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	2
4,25	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	5	2
3,27	C ₁₈ H ₃₀	2719-62-2	Benzene, (1-pentylheptyl)-	4	2
3,06	C ₁₈ H ₁₂	56-55-3	Benz[a]anthracene	6	2
2,46	C ₁₁ H ₁₀	91-57-6	Naphthalene, 2-methyl-	6	2
1,49	C ₁₁ H ₁₀	90-12-0	Naphthalene, 1-methyl-	6	2
1,28	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
		843-55-0	bisfenol Z	3	1
		13595-25-0	bisphenol M	3	1
		80-09-1	bisphenol S	1	1
		5835-26-7	isopimaric acid	4	2
		123-08-0	4-hydroxybenzaldehyde	7	2

Table 22: Sediment Norway

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
166,10	C ₂₄ H ₃₈ O ₄	-	Phthalic acid, di(2-propylpentyl) ester	1	2
164,41	C ₁₆ H ₁₀	206-44-0	Fluoranthene	6	2
163,97	C ₁₆ H ₁₀	129-00-0	Pyrene	6	2
149,78	C ₈ H ₁₀ O ₂	122-99-6	Ethanol, 2-phenoxy-	3	2
101,70	C ₂₀ H ₁₂	205-99-2	Benzo[b]fluoranthene	4	2
91,70	C ₂₀ H ₁₂	192-97-2	Benzo[e]pyrene	5	2
84,46	C ₁₈ H ₁₂	217-59-4	Triphenylene	6	2
75,89	C ₁₄ H ₁₀	85-01-8	Phenanthrene	6	2
58,79	C ₁₈ H ₁₂	56-55-3	Benz[a]anthracene	6	2
50,76	C ₂₀ H ₁₂	50-32-8	Benzo[a]pyrene	5	2
39,93	C ₂₀ H ₁₂	198-55-0	Perylene	5	2
37,88	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
37,30	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
24,14	C ₇ H ₇ NO ₂	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
23,53	C ₁₄ H ₁₀	120-12-7	Anthracene	6	2
23,12	C ₁₁ H ₁₆ O ₂	15356-74-8	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	5	2
22,28	C ₉ H ₁₂ O ₂	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
21,46	C ₁₅ H ₁₂	-	Phenanthrene, methyl-	1	3
21,43	C ₁₆ H ₁₀ O	205-39-0	Benzo(b)naphtho(1,2-d)furan	5	3
20,52	C ₁₉ H ₁₄	82979-72-4	8,9-Dihydro-7H-cyclopenta[a]pyrene	5	3
20,21	C ₁₇ H ₁₂	243-17-4	11H-Benzo[b]fluorene	5	2
16,14	C ₁₂ H ₈ O	132-64-9	Dibenzofuran	5	2
15,72	C ₁₃ H ₁₆ O	55591-10-1	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-	4	3
14,52	C ₁₆ H ₁₀ S	205-43-6	Benzo[b]naphtho[1,2-d]thiophene	5	2
13,93	C ₁₈ H ₁₈	66552-97-4	2-Isopropyl-10-methylphenanthrene	5	3
13,91	C ₁₆ H ₁₆	7694-30-6	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	5	2
11,42	C ₁₆ H ₁₂	6232-48-0	Acphenanthrylene, 4,5-dihydro-	5	2
9,83	C ₁₅ H ₁₀	83469-43-6	6H-Cyclobuta[jk]phenanthrene	5	2
9,69	C ₁₆ H ₁₀ O	200-23-7	Benzo[k]xanthene	4	3
9,00	C ₁₁ H ₁₀	91-57-6	Naphthalene, 2-methyl-	6	2
8,75	C ₁₆ H ₁₄	3674-69-9	Phenanthrene, 4,5-dimethyl-	5	2
8,28	C ₉ H ₇ NO	487-89-8	1H-Indole-3-carboxaldehyde	3	2
8,04	C ₁₄ H ₈ O ₂	84-65-1	9,10-Anthracenedione	5	2
7,76	C ₁₂ H ₁₂	-	Naphthalene, dimethyl-	10	3
7,63	C ₁₉ H ₁₂	50861-05-7	9H-Cyclopenta[a]pyrene	5	2
7,54	C ₁₃ H ₁₀ O	3218-36-8	[1,1'-Biphenyl]-4-carboxaldehyde	4	2
7,47	C ₂₁ H ₁₄	239-85-0	13H-Dibenzo[a,h]fluorene	5	3
6,89	C ₁₃ H ₁₀	86-73-7	Fluorene	4	2
6,13	C ₁₁ H ₁₀	90-12-0	Naphthalene, 1-methyl-	6	2
5,87	C ₁₂ H ₁₂	-	Naphthalene, dimethyl-	10	3
5,56	C ₁₅ H ₁₂	27410-55-5	8,9-Dihydrocyclopenta[def]phenanthrene	5	3
5,50	C ₁₃ H ₈ O	548-39-0	1H-Phenalen-1-one	4	2
4,72	C ₁₇ H ₁₀ O	82-05-3	7H-Benz[de]anthracen-7-one	4	2
4,66	C ₁₇ H ₁₆	3674-73-5	Phenanthrene, 2,3,5-trimethyl-	4	2
4,50	C ₁₅ H ₁₂	832-64-4	Phenanthrene, 4-methyl-	4	2
4,45	C ₁₃ H ₁₀ O	92-83-1	9H-Xanthene	5	2
4,41	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
3,98	C ₁₈ H ₁₂	195-19-7	Benzo[c]phenanthrene	5	2
3,97	C ₈ H ₅ Br ₂ N	-	2-Bromo-6-(3-bromo-prop-1-ynyl)-pyridine	2	3
3,88	C ₁₆ H ₁₀ S	227-86-1	Anthra(1,2-b)thiophene	3	3
3,80	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
3,80	C ₁₅ H ₈ O	5737-13-3	Cyclopenta(def)phenanthrenone	4	2
3,54	C ₁₈ H ₁₀ O	191-37-7	Naphtho[2,1,8,7-klmn]xanthene	4	3
3,49	C ₈ H ₇ NS ₂	615-22-5	Benzo[thiazole, 2-(methylthio)-	2	2
3,24	C ₂₀ H ₁₄	612-78-2	2,2'-Binaphthalene	3	3
3,18	C ₁₃ H ₁₄	829-26-5	Naphthalene, 2,3,6-trimethyl-	4	2
2,87	C ₁₆ H ₁₄	1576-67-6	Phenanthrene, 3,6-dimethyl-	5	2
2,77	C ₁₆ H ₁₁ N	-	11H-Benzo[a]carbazole (isomer)	7	3
2,60	C ₁₆ H ₁₀ S	239-35-0	Benzo[b]naphtho[2,1-d]thiophene	3	2
		92612-52-7	PFHxA	4	2

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
		754-91-6	FOSA	1	2
		135984-67-7	4:2 FTAL	1	2
		620-92-8	4,4-BPF	1	2
		5835-26-7	isopimaric acid	4	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2

Table 23: Sediment Greenland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
16,22	C ₁₀ H ₁₆	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	4	2
34,05	C ₂₃ H ₃₆ O ₄	-	Phthalic acid, hept-3-yl octyl ester	6	2
24,34	C ₁₂ H ₆ Cl ₄	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
21,24	C ₇ H ₅ NS	95-16-9	Benzothiazole	6	2
21,16	C ₁₃ H ₁₀ O	119-61-9	Benzophenone	7	2
9,05	C ₇ H ₇ NO ₂	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
8,63	C ₁₂ H ₆ Cl ₄	-	1,1'-Biphenyl, 2,2',5,5'-tetramethyl- (isomer)	3	3
7,54	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
7,15	C ₁₆ H ₂₀	24157-81-1	2,6-Diisopropyl-naphthalene	3	2
6,71	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	4	3
5,94	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	5	2
5,92	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
4,53	C ₂₂ H ₃₆ O ₂	-	Benzoic acid, pentadecyl ester	5	3
4,31	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	5	3
3,26	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2

Table 24: Sediment Faroe Islands

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
182,68	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	6	2
56,76	C20H12	205-99-2	Benzo[b]fluoranthene	4	2
43,37	C13H10O	119-61-9	Benzophenone	7	2
39,51	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	5	2
37,21	C22H12	193-39-5	Indeno[1,2,3-cd]pyrene	4	2
32,49	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	6	3
30,45	C7H5NS	95-16-9	Benzo[thiazole]	6	2
25,63	C20H12	192-97-2	Benzo[e]pyrene	5	2
25,32	C20H12	50-32-8	Benzo[a]pyrene	5	2
22,65	C16H10	206-44-0	Fluoranthene	6	2
16,94	C18H12	217-59-4	Triphenylene	6	2
16,18	C16H20	24157-81-1	2,6-Diisopropyl-naphthalene	3	2
15,47	C22H12	193-43-1	Indeno[1,2,3-cd]fluoranthene	4	2
14,82	C18H30	2719-62-2	Benzene, (1-pentylheptyl)-	4	2
14,45	C14H10	85-01-8	Phenanthrene	6	2
13,22	C18H18	66552-97-4	2-Isopropyl-10-methylphenanthrene	5	3
12,45	C16H10	129-00-0	Pyrene	6	2
10,29	C16H16	7694-30-6	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	5	2
9,54	C19H14	82979-72-4	8,9-Dihydro-7H-cyclopenta[a]pyrene	5	3
8,81	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	4	3
8,71	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	6	2
8,40	C20H16	35187-19-0	4,12-Dimethylbenz[a]anthracene	4	3
8,32	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
8,18	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	5	2
8,00	C14H10	120-12-7	Anthracene	6	2
7,41	C9H14O6	102-76-1	Triacetin	3	2
7,30	C30H50	1615-91-4	Diploptene	4	3
7,19	C18H12	56-55-3	Benzo[a]anthracene	6	2
7,07	C15H28	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	3	3
6,55	C10H8	91-20-3	Naphthalene	4	2
6,44	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	6	2
6,38	C18H12	195-19-7	Benzo[c]phenanthrene	5	2
6,15	C17H16	3674-73-5	Phenanthrene, 2,3,5-trimethyl-	4	2
6,11	C18H26O	1222-05-5	Galaxolide	2	2
5,78	C17H28	4537-15-9	Benzene, (1-butylheptyl)-	3	2
5,49	C20H12	198-55-0	Perylene	5	2
5,44	C8H10O2	122-99-6	Ethanol, 2-phenoxy-	3	2
5,30	C17H12	199-94-0	7H-Benzo[de]anthracene	4	3
5,12	C18H14S	24964-12-3	Benzo[b]naphtho[2,3-d]thiophene, 7,8-dimethyl-	3	3
4,95	C15H12	27410-55-5	8,9-Dihydrocyclopenta[def]phenanthrene	5	3
4,54	C15H10	83469-43-6	6H-Cyclobuta[jk]phenanthrene	5	2
3,99	C16H14	3674-69-9	Phenanthrene, 4,5-dimethyl-	5	2
3,96	C20H12	205-82-3	Benzo[j]fluoranthene	4	2
3,51	C21H36	641-85-0	Allopregnane	3	3
3,46	C17H12	243-17-4	11H-Benzo[b]fluorene	5	2
3,44	C10H14	527-53-7	Benzene, 1,2,3,5-tetramethyl-	2	2
3,35	C12H8O	132-64-9	Dibenzofuran	5	2
3,20	C7H6O2	65-85-0	Benzoic acid	1	2
3,16	C15H12	832-69-9	Phenanthrene, 1-methyl-	3	2
2,90	C12H12	-	Naphthalene, dimethyl-	10	3
2,87	C18H22	6566-19-4	10,18-Bisnorabieta-5,7,9(10),11,13-pentaene	3	3
2,74	C18H10O	191-37-7	Naphtho[2,1,8,7-klmn]xanthene	4	3
2,71	C11H10	91-57-6	Naphthalene, 2-methyl-	6	2
2,69	C11H16O2	15356-74-8	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	5	2
2,56	C21H14	63104-32-5	10-Methylbenzo(a)pyrene	4	3
2,56	C21H14	239-85-0	13H-Dibenzo[a,h]fluorene	5	3
2,55	C20H32O2	-	Benzoic acid, tridecyl ester	4	3
2,47	C12H12	-	Naphthalene, dimethyl-	10	3
2,44	C11H10	90-12-0	Naphthalene, 1-methyl-	6	2
2,24	C8H5Br2N	-	2-Bromo-6-(3-bromo-prop-1-ynyl)-pyridine	2	3
2,15	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	3	2
2,15	C22H36O2	-	Benzoic acid, pentadecyl ester	5	3
2,05	C16H10S	205-43-6	Benzo[b]naphtho[1,2-d]thiophene	5	2

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
2,05	C ₇ H ₉ NO ₂	20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	7	3
2,02	C ₁₈ H ₂₈ O ₂	6316-30-9	Benzoic acid, undecyl ester	5	3
2,02	C ₂₄ H ₃₈ O ₄	6422-86-2	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2	3
2,01	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
2,00	C ₁₆ H ₁₄	1576-67-6	Phenanthrene, 3,6-dimethyl-	5	2
1,90	C ₁₃ H ₈ O	548-39-0	1H-Phenalen-1-one	4	2
1,90	C ₁₇ H ₁₂ S	-	2-Methylbenzo[b]naphtho[2,1-d]thiophene	3	3
1,90	C ₁₅ H ₁₂	832-71-3	Phenanthrene, 3-methyl-	4	2
1,81	C ₁₃ H ₁₄	829-26-5	Naphthalene, 2,3,6-trimethyl-	4	2
1,73	C ₁₆ H ₁₀ O	205-39-0	Benzo(b)naphtho(1,2-d)furan	5	3
1,68	C ₁₈ H ₁₀	203-12-3	Benzo[ghi]fluoranthene	3	2
1,60	C ₁₀ H ₁₄	488-23-3	Benzene, 1,2,3,4-tetramethyl-	3	2
1,55	C ₁₁ H ₂₀	2958-76-1	Naphthalene, decahydro-2-methyl-	2	2
1,54	C ₂₁ H ₁₄	241-28-1	8H-Indeno[2,1-b]phenanthrene	4	3
1,46	C ₁₅ H ₂₂	483-77-2	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	3	2
1,45	C ₁₃ H ₁₀	86-73-7	Fluorene	4	2
1,40	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
1,39	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	6	2
1,38	C ₁₉ H ₁₂	50861-05-7	9H-Cyclopenta[a]pyrene	5	2
1,32	C ₁₃ H ₁₀ O	3218-36-8	[1,1'-Biphenyl]-4-carboxaldehyde	4	2
1,27	C ₁₆ H ₁₂	6232-48-0	Acephenanthrylene, 4,5-dihydro-	5	2
1,23	C ₁₃ H ₁₀ O	92-83-1	9H-Xanthene	5	2
1,17	C ₆ H ₅ BrO	591-20-8	Phenol, 3-bromo-	2	2
1,15	C ₁₅ H ₁₂	832-64-4	Phenanthrene, 4-methyl-	4	2
1,12	C ₁₄ H ₁₄	613-33-2	4,4'-Dimethylbiphenyl	3	2
1,10	C ₁₆ H ₁₁ N	-	11H-Benzo[a]carbazole (isomer)	7	3
1,02	C ₈ H ₈ O ₂	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	3	2
1,02	C ₁₆ H ₁₀ O	243-42-5	Benzo[b]naphtho[2,3-d]furan	4	3
0,95	C ₁₄ H ₁₂ S	1136-85-2	3,7-Dimethyldibenzothiophene	3	2
0,90	C ₁₄ H ₈ O ₂	84-65-1	9,10-Anthracenedione	5	2
0,90	C ₁₂ H ₅ Cl ₅	32598-14-4	1,1'-Biphenyl, 2,3,3',4,4'-pentachloro-	2	2
0,84	C ₁₇ H ₁₂	-	7H-Benzo[c]fluorene (isomer)	13	3
0,79	C ₁₂ H ₁₂ O ₅	5062-30-6	Phenacylidene diacetate	2	2
0,77	C ₇ H ₇ NO ₂	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	6	3
0,77	C ₁₁ H ₁₈ O ₄	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	3	2
0,74	C ₁₆ H ₁₁ N	-	11H-Benzo[a]carbazole (isomer)	7	3
0,63	C ₁₅ H ₈ O	5737-13-3	Cyclopenta(def)phenanthrenone	4	2
0,62	C ₂₁ H ₄₄ O ₂ Si	18748-91-9	Octadecanoic acid, trimethylsilyl ester	1	2
0,56	C ₁₂ H ₅ Cl ₅	55215-17-3	1,1'-Biphenyl, 2,2',3,4,6-Pentachloro-	1	2
0,54	C ₁₃ H ₁₂	643-93-6	1,1'-Biphenyl, 3-methyl-	3	2
	C ₁₅ H ₁₄ N ₄ O ₂ S	526-08-9	sulfaphenazole	1	2
	C ₅ H ₁₀ O ₄ S	30618-84-9	mercaptoacetic acid, monoester with propane-1,2,3-triol		
	C ₄ H ₁₀ O ₃ S	2386-47-2	1-butan-sulfonic acid	1	2
	C ₇ H ₆ O ₂	100-83-4	3-hydroxybenzaldehyde	1	2
	C ₇ H ₆ O ₂	65-85-0	Benzoic acid	2	2
	C ₉ H ₁₄ O ₄	86273-46-3	2-(2-Vinyloxyethoxy)ethyl acrylate	1	2
	C ₁₆ H ₁₀ ClN ₃ O ₃	2814-77-9	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	1	2
		5835-26-7	isopimaric acid	4	2
		123-08-0	4-hydroxybenzaldehyde	7	2
		1074-86-8	4-formyl indole	6	2
		92612-52-7	PFHxA	4	2

Table 25: Fish Finland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
1673,34	C ₁₄ H ₂₆ O ₂	544-64-9	Myristoleic acid	6	2
600,59	C ₁₇ H ₃₆ O ₂ Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
588,59	C ₈ H ₁₂ O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
484,62	C ₁₉ H ₄₀ O ₂ Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
472,13	C ₂₄ H ₃₈ O ₄	-	Phthalic acid, di(6-methylhept-2-yl) ester	2	2
313,62	C ₂₃ H ₄₀ O ₃	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
235,49	C ₁₇ H ₃₄ O	-	Hexadecanal, methyl-	2	2
209,20	C ₁₈ H ₃₈ O ₂ Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
181,78	C ₁₇ H ₂₅ NO ₄	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	5	2
180,42	C ₇ H ₅ NS	95-16-9	Benzothiazole	5	2
108,22	C ₁₁ H ₁₈ O ₄	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
105,74	C ₇ H ₆ O ₂	65-85-0	Benzoic acid	7	2
101,96	C ₉ H ₁₂ O ₂	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	4	2
97,54	C ₉ H ₁₀ O ₃	10139-84-1	2',4'-Dihydroxy-3'-methylacetophenone	5	2
92,87	C ₁₄ H ₁₄ O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	3	2
74,40	C ₉ H ₁₀ O ₂	140-11-4	Acetic acid, phenylmethyl ester	3	2
61,54	C ₁₀ H ₁₄ O ₂	1948-33-0	t-Butylhydroquinone	5	2
60,51	C ₂₁ H ₃₆ O ₃	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
44,09	C ₈ H ₆ O ₂	1074-12-0	Phenylglyoxal	5	2
31,71	C ₁₂ H ₂₄ O ₃	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
25,94	C ₁₂ H ₁₂ O ₅	5062-30-6	Phenacylidene diacetate	4	2
23,76	C ₁₄ H ₁₄	611-43-8	1,1'-Biphenyl, 2,3'-dimethyl-	3	2
19,30	C ₅ H ₉ NO ₂	4394-85-8	N-Formylmorpholine	7	2
16,88	C ₆ H ₈ O ₃	29393-32-6	2(3H)-Furanone, 5-acetyldihydro-	3	2
15,65	C ₁₂ H ₆ Cl ₄	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
12,51	C ₁₄ H ₁₄	611-61-0	1,1'-Biphenyl, 2,4'-dimethyl-	3	2
8,65	C ₁₄ H ₁₄	613-33-2	4,4'-Dimethylbiphenyl	3	2
8,26	C ₉ H ₁₈ Cl ₃ O ₄ P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	5	2
7,88	C ₁₂ H ₄ Cl ₆	74472-43-8	2,3,3',4,5',6-Hexachloro-1,1'-biphenyl	4	2
6,49	C ₁₂ H ₄ Cl ₆	52663-72-6	1,1'-Biphenyl, 2,3',4,4',5,5'-hexachloro-	2	2
5,77	C ₈ H ₁₀ O ₂	122-99-6	Ethanol, 2-phenoxy-	1	2
4,91	C ₂₀ H ₃₂ O ₂	-	Benzoic acid, tridecyl ester	1	3
4,83	C ₁₆ H ₂₀	24157-81-1	2,6-Diisopropyl-naphthalene	2	2
4,73	C ₁₂ H ₅ Cl ₅	55215-17-3	1,1'-Biphenyl, 2,2',3,4,6-Pentachloro-	3	2
4,62	C ₉ H ₁₀ O ₂	70-70-2	Paroxypropione	5	2
3,85	C ₆ H ₁₁ NO ₂	1696-20-4	Morpholine, 4-acetyl-	2	3
2,66	C ₁₃ H ₁₆	30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	3	2
2,25	C ₁₂ H ₃ Cl ₇	35065-30-6	1,1'-Biphenyl, 2,2',3,3',4,4',5'-heptachloro-	2	2
Qualitative	C ₆ H ₄ Br ₂ O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C ₇ H ₅ Br ₃	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C ₆ H ₃ Br ₃ O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C ₁₂ H ₅ Cl ₅	31508-00-6	PCB-118	7	2
Qualitative	C ₁₂ H ₄ Cl ₆	35065-27-1	PCB-153	7	2
Qualitative	C ₁₂ H ₅ Cl ₅	32598-14-4	PCB-105	5	2
Qualitative	C ₁₂ H ₄ Cl ₆	35065-28-2	PCB-138	7	2
Qualitative	C ₁₂ H ₄ Cl ₆	52663-72-6	PCB-167	7	2
Qualitative	C ₁₂ H ₄ Cl ₆	38380-08-4	PCB-156	7	2
Qualitative	C ₁₂ H ₄ Cl ₆	69782-90-7	PCB-157	7	2
Qualitative	C ₁₂ H ₃ Cl ₇	35065-29-3	PCB-180	7	2
Qualitative	C ₁₂ H ₆ Br ₄ O	189084-61-5	2,3',4',6-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C ₁₂ H ₃ Cl ₇	35065-30-6	PCB-170	7	2
Qualitative	C ₁₂ H ₃ Cl ₇	39635-31-9	PCB-189	7	2
Qualitative	C ₁₂ H ₅ Br ₅ O	93703-48-1	2,2',3,4,4',6-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C ₁₂ H ₂ Cl ₈	52663-78-2	PCB-195	7	3
Qualitative	C ₁₂ H ₂ Cl ₈	35694-08-7	PCB-194	7	2
Qualitative	C ₁₂ H ₅ Br ₅ O	60348-60-9	2,2',4,4',6-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C ₁₂ HCl ₉	40186-72-9	PCB-206	7	2
Qualitative	C ₁₂ Cl ₁₀	2051-24-3	PCB-209	7	2
Qualitative	C ₁₂ H ₄ Br ₆ O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C ₁₅ H ₁₂ Br ₄ O ₂	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
Qualitative	C ₉ H ₁₀ O ₃	6161-65-5	2-methoxy-6-methylbenzoic acid	1	3
Qualitative	C ₁₀ H ₁₆ N ₂ O ₄	10543-57-4	N,N'-ethylenebis[N'-acetylacetamide]	1	3
Qualitative	C ₅ H ₄ N ₄ O ₂	2465-59-0	oxypurinol	1	3

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
Qualitative	C ₈ H ₁₁ NO ₃	65-23-6	pyridoxine	1	3
Qualitative	C ₁₀ H ₁₃ N ₅ O ₅	118-00-3	Guanosine	1	3
Qualitative	C ₁₀ H ₁₂ N ₄ O ₅	16220-07-8	Allopurinol riboside	2	3
Qualitative	C ₁₂ H ₁₅ N ₅ O ₅	75128-73-3	2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl)methoxy]ethyl acetate	2	3
Qualitative	C ₁₁ H ₂₀ N ₂ O ₅	27317-69-7	N-[N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl]-L-alanine	1	3
Qualitative	C ₁₆ H ₃₂ O ₂	57-10-3	Hexadecanoic acid	1	3
Qualitative	C ₁₆ H ₁₀ ClN ₃ O ₃	2814-77-9	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	1	3
Qualitative	C ₂₂ H ₃₂ O ₂	127-47-9	retinyl acetate	1	3
Qualitative	C ₈ H ₁₇ O ₃ S	1763-23-1	Perfluorooctane sulfonate (PFOS) (Acid)	1	3
Qualitative	C ₅ H ₄ N ₄ O	315-30-0	allopurinol	1	3
Qualitative	C ₈ H ₁₈ N ₂ O ₄ S	7365-45-9	4-(2-hydroxyethyl)piperazin-1-ylethanesulphonic acid	1	3
Qualitative	C ₁₈ H ₃₆ O ₂	57-11-4	Octadecanoic acid	1	3
Qualitative	C ₁₉ H ₃₈ O ₂	68517-10-2	methyl isostearate	1	3
Qualitative	C ₁₉ H ₃₈ O ₂	142-91-6	Hexadecanoic acid, 1-methylethyl ester	1	3
Qualitative	C ₁₉ H ₃₈ O ₂	112-61-8	methyl stearate	1	3
Qualitative	C ₈ H ₂₁ NOSi ₂	10416-59-8	trimethylsilyl N-trimethylsilylacetamidate	1	3
Qualitative	C ₆ H ₉ NO ₂	72291-30-6	Propanoic acid, 2-cyano-2-methyl-, methyl ester	1	3
Qualitative	C ₁₁ H ₁₂ N ₂ O ₂	73-22-3	Tryptophan	1	3
Qualitative	C ₉ H ₁₄ O ₃	2455-24-5	tetrahydrofurfuryl methacrylate	1	3
Qualitative	C ₃₁ H ₄₈ O ₂ S ₂	23288-49-5	probuco	1	3
Qualitative	C ₆ H ₉ N ₃ O ₂	4998-57-6	histidine	1	3
Qualitative	C ₄ H ₆ O ₄	110-15-6	succinic acid	1	3
Qualitative	C ₁₂ H ₈ O ₄	298-81-7	methoxsalen	1	3
Qualitative	C ₁₂ H ₂₄ N ₂ O ₃	6425-39-4	2,2'-dimorpholinyl diethyl ether	1	3
Qualitative	C ₂₆ H ₄₅ NO ₇ S	81-24-3	taurocholic acid	2	3
Qualitative	C ₅ H ₉ NO ₂	923-02-4	N-(hydroxymethyl)methacrylamide	1	3
Qualitative	C ₅ H ₉ NO ₂	7646-67-5	N-(2-hydroxyethyl)prop-2-enamide	1	3
Qualitative	C ₅ H ₉ NO ₂	81778-07-6	4,4-dimethyl-1,2-oxazolidin-3-one	1	3
Qualitative	C ₅ H ₉ NO ₂	14205-39-1	methyl 3-aminocrotonate	1	3
		474511-07-4	PFNS	2	2
		171978-95-3	PFDoDA	2	2
		39108-34-4	8:2 FTS	1	2
		355-46-4	PFHxS	2	2
		106-44-5	p-cresol	2	3
		550-24-3	embelin	2	3
		352-21-6	aminohydroxybutyric acid	2	3
		123-08-0	4-hydroxybenzaldehyde	6	3
		1074-86-8	4-formyl indole	6	3
		66621-73-6	2-pyrimidine acetic acid	3	3

Table 26: Fish Sweden

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3342,56	C14H26O2	544-64-9	Myristoleic acid	6	2
1717,17	C17H25NO4	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	5	2
888,20	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
696,89	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
588,78	C23H40O3	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
318,22	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
249,74	C7H5NS	95-16-9	Benzothiazole	5	2
249,70	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	2	2
207,32	C9H10O3	10139-84-1	2',4'-Dihydroxy-3'-methylacetophenone	5	2
205,96	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	4	2
148,81	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
147,46	C9H10O2	122-46-3	m-Cresyl acetate	1	2
146,65	C7H6O2	65-85-0	Benzoic acid	7	2
124,83	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	3	2
104,67	C21H36O3	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
62,20	C10H14O2	1948-33-0	t-Butylhydroquinone	5	2
55,45	C6H8O3	29393-32-6	2(3H)-Furanone, 5-acetyldihydro-	3	2
48,03	C9H8O	83-33-0	1H-Inden-1-one, 2,3-dihydro-	2	2
42,96	C18H26O	1222-05-5	Galaxolide	4	2
42,72	C14H14	611-43-8	1,1'-Biphenyl, 2,3'-dimethyl-	3	2
36,38	C12H12O5	5062-30-6	Phenacylidene diacetate	4	2
26,79	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
26,21	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	3	2
23,19	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
22,74	C9H10O2	70-70-2	Paroxypropione	5	2
18,94	C14H14	611-61-0	1,1'-Biphenyl, 2,4'-dimethyl-	3	2
18,63	C8H6O2	1074-12-0	Phenylglyoxal	5	2
16,57	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
15,70	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
13,27	C7H9NOS	934-34-9	2(3H)-Benzothiazolone	3	3
12,48	C7H8O2	504-15-4	Orcinol	2	2
11,66	C14H14	613-33-2	4,4'-Dimethylbiphenyl	3	2
8,19	C8H8O2	582-24-1	Ethanone, 2-hydroxy-1-phenyl-	1	2
7,47	C9H8O3	7310-95-4	2-Hydroxy-5-methylisophthalaldehyde	1	2
7,30	C12H5Cl5	55215-17-3	1,1'-Biphenyl, 2,2',3,4,6-Pentachloro-	3	2
6,18	C13H16	30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	3	2
5,93	C12H4Cl6	74472-43-8	2,3,3',4,5',6-Hexachloro-1,1'-biphenyl	4	2
5,44	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	5	2
3,45	C17H34O	55019-46-0	Hexadecanal, 2-methyl-	3	2
1,14	C17H34O	-	Hexadecanal, methyl-	2	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H5Cl5	31508-00-6	PCB-118	7	2
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H5Cl5	32598-14-4	PCB-105	5	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2
Qualitative	C12Cl10	2051-24-3	PCB-209	7	2
Qualitative	C12H4Br6O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C15H12Br4O2	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
Qualitative	C23H32N2O4	243973-20-8	pinoxaden	1	3

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
Qualitative	C ₂₄ H ₃₄ O ₄	82543-17-7		1	3
Qualitative	C ₉ H ₁₇ NO ₃ S	35130-97-3	Tropine-3-mesylate	1	3
Qualitative	C ₁₅ H ₁₂ N ₂ O ₂	36507-30-9	10,11-Epoxy carbamazepine	1	3
Qualitative	C ₂₅ H ₃₇ NO ₄	89365-50-4		1	3
Qualitative	C ₂₃ H ₁₅ N ₃ O	380917-97-5		1	3
Qualitative	C ₂₀ H ₃₂ O ₂	34434-80-5		2	3
		474511-07-4	PFNS	2	2
	C ₁₂ HF ₂₃ O ₂	171978-95-3	PFDODA	2	2
		80705-13-1	4:3 Acid	1	2
		355-46-4	PFHxS	2	2
		106-44-5	p-cresol	2	3
		352-21-6	aminohydroxybutyric acid	2	3
		123-08-0	4-hydroxybenzaldehyde	6	3
		1074-86-8	4-formyl indole	6	3
		60-32-2	aminocaproic acid	4	3
		66621-73-6	2-pyrimidine acetic acid	3	3

Table 27: Fish Denmark

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3070,12	C14H26O2	544-64-9	Myristoleic acid	6	2
1055,79	C23H40O3	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
698,51	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
615,66	C21H36O3	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
481,65	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
454,13	C17H25NO4	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	5	2
426,38	C7H5NS	95-16-9	Benzothiazole	5	2
318,84	C24H38O4	-	Phthalic acid, di(2-propylpentyl) ester	3	2
267,72	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
241,15	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
193,72	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	4	2
192,92	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
181,47	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
113,86	C16H33NO	629-54-9	Hexadecanamide	4	2
87,73	C10H14O2	1948-33-0	t-Butylhydroquinone	5	2
75,30	C9H10O2	140-11-4	Acetic acid, phenylmethyl ester	3	2
57,57	C12H12O5	5062-30-6	Phenacylidene diacetate	4	2
51,26	C7H5NOS	934-34-9	2(3H)-Benzothiazolone	3	3
50,73	C11H16O2	17092-92-1	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	3	2
44,01	C7H6O2	65-85-0	Benzoic acid	7	2
43,64	C9H10O3	10139-84-1	2',4'-Dihydroxy-3'-methylacetophenone	5	2
42,39	C9H10O2	70-70-2	Paroxypropione	5	2
41,05	C9H8O	83-33-0	1H-Inden-1-one, 2,3-dihydro-	2	2
39,21	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
37,95	C14H14	611-43-8	1,1'-Biphenyl, 2,3'-dimethyl-	3	2
37,70	C7H8O2	504-15-4	Orcinol	2	2
31,78	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	3	2
29,24	C14H8N2S2	4271-09-4	2,2'-Bibenzothiazole	1	3
28,86	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
26,56	C8H6O2	1074-12-0	Phenyglyoxal	5	2
16,96	C14H14	611-61-0	1,1'-Biphenyl, 2,4'-dimethyl-	3	2
14,70	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
13,57	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	4	2
10,53	C14H14	613-33-2	4,4'-Dimethylbiphenyl	3	2
10,12	C6H8O3	29393-32-6	2(3H)-Furanone, 5-acetyldihydro-	3	2
9,73	C7H7NO2	21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	1	3
6,25	C6H11NO2	1696-20-4	Morpholine, 4-acetyl-	2	3
5,41	C10H21NO	1118-92-9	Octanamide, N,N-dimethyl-	2	2
4,13	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	5	2
4,09	C10H8	91-20-3	Naphthalene	1	2
3,90	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	5	2
3,59	C10H22O3	29911-28-2	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	1	3
3,33	C9H8O	4432-63-7	2-Phenylpropenal	4	2
3,26	C11H10	91-57-6	Naphthalene, 2-methyl-	1	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H5Cl5	31508-00-6	PCB-118	7	2
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H5Cl5	32598-14-4	PCB-105	5	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6'-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6'-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
Qualitative	C ₁₂ Cl ₁₀	2051-24-3	PCB-209	7	2
Qualitative	C ₁₂ H ₄ Br ₆ O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C ₁₅ H ₁₂ Br ₄ O ₂	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
		76811-98-8	Benzeneacetic acid, 4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-α,α-dimethyl-		
		61432-55-1	Dimepiperate	1	3
		58-63-9	Inosine	2	3
		16220-07-8	Allopurinol riboside	2	3
		2387-59-9	carbocysteine	1	3
		34306-42-8	(S)-2-((tert)-butoxycarbonyl)amino)butanoic acid		
		123-08-0	4-hydroxybenzaldehyde	6	3
		1074-86-8	4-formyl indole	6	3
		66621-73-6	2-pyrimidine acetic acid	3	3

Table 28: Fish Iceland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
17849,44	C12H22	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	2	3
7225,30	C23H40O3	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
3814,04	C11H20	2958-76-1	Naphthalene, decahydro-2-methyl-	2	2
3708,65	C14H26O2	544-64-9	Myristoleic acid	6	2
2687,54	C24H38O4	-	Phthalic acid, di(2-propylpentyl) ester	3	2
1889,93	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
1593,13	C11H20	-	trans-Decalin, 2-methyl-	2	2
1520,04	C21H36O3	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
1378,49	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
1264,38	C17H28	4537-15-9	Benzene, (1-butylheptyl)-	2	2
1038,66	C12H22	66660-41-1	2-Ethyldecahydronaphthalene, (Z,E)-	2	2
862,66	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
800,29	C18H30	2719-62-2	Benzene, (1-pentylheptyl)-	2	2
458,16	C16H33NO	629-54-9	Hexadecanamide	4	2
457,56	C18H37NO	-	Octadecanamide (branched)	1	3
308,52	C15H28	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	2	2
246,38	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
225,80	C17H25NO4	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	5	2
99,43	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	4	2
86,31	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
85,27	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
83,78	C12H4Cl6	74472-43-8	2,3,3',4,5',6-Hexachloro-1,1'-biphenyl	4	2
78,42	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
67,62	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
62,68	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
60,34	C18H26O	1222-05-5	Galaxolide	4	2
57,73	C7H6O2	65-85-0	Benzoic acid	7	2
46,51	C12H5Cl5	32598-14-4	1,1'-Biphenyl, 2,3,3',4,4'-pentachloro-	2	2
46,28	C16H20	24157-81-1	2,6-Diisopropyl-naphthalene	2	2
32,89	C15H22	483-77-2	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	1	2
28,34	C10H21NO	1118-92-9	Octanamide, N,N-dimethyl-	2	2
26,99	C13H10O	119-61-9	Benzophenone	1	2
26,69	C11H16O2	17092-92-1	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	3	2
20,12	C9H8O	4432-63-7	2-Phenylpropenal	4	2
14,40	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
7,99	C9H10O3	10139-84-1	2',4'-Dihydroxy-3'-methylacetophenone	5	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H8Br2O	147217-71-8	2,4'-Dibromodiphenyl ether (PBDE#7)	4	2
Qualitative	-	-	Natural product, Br3Cl3, probably monoterpene	4	5
Qualitative	C12H5Cl5	31508-00-6	PCB-118	7	2
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H5Cl5	32598-14-4	PCB-105	5	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2
Qualitative	C12Cl10	2051-24-3	PCB-209	7	2
Qualitative	C12H4Br6O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C15H12Br4O2	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
	C14H24N2O4	187227-45-8	Oseltamivircarbonsäure	1	3
	C15H12N2O3	2784-27-2	5-(4-hydroxyphenyl)-5-phenylhydantoin	1	3
	C14H29NO7Si	192389-48-3	diethyl N-[3-(trimethoxysilyl)propyl]aspartate	1	3

Continued				
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix ID Level
	C ₉ H ₁₆ O ₃	65593-73-9	Methyl (cyclohexyloxy)acetate	1 3
	C ₁₇ H ₂₄ O	13171-00-1	Celestolide	1 3
	C ₁₀ H ₁₀ O	529-34-0	Tetralinone	1 3
	C ₁₅ H ₁₄ O ₆	154-23-4	catechin	1 3
		843-55-0	bisfenol Z	3 1
		1478-61-1	hexafluoroBPA (bisfenol AF)	3 1
		123-08-0	4-hydroxybenzaldehyd	6 2
		1074-86-8	4-formyl indole	6 3
		60-32-2	aminocaproic acid	4 3

Table 29: Fish Norway

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3442,34	C14H26O2	544-64-9	Myristoleic acid	6	2
2484,13	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
1925,69	C7H5NS	95-16-9	Benzothiazole	5	2
1691,36	C23H40O3	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
549,96	C7H6O2	65-85-0	Benzoic acid	7	2
545,81	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	3	2
469,71	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
458,54	C7H5NS	272-16-2	1,2-Benzisothiazole	3	2
442,79	C21H36O3	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
440,55	C23H36O4	-	Phthalic acid, hept-3-yl octyl ester	2	2
424,42	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
415,40	C7H5NS2	149-30-4	2-Mercaptobenzothiazole	1	2
326,98	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
166,29	C12H4Cl6	74472-43-8	2,3,3',4,5',6'-Hexachloro-1,1'-biphenyl	4	2
148,49	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
144,94	C16H33NO	629-54-9	Hexadecanamide	4	2
131,82	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
121,41	C18H26O	1222-05-5	Galaxolide	4	2
117,15	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	4	2
104,92	C14H14O	19578-70-2	Benzene, 1-methyl-2-(phenylmethoxy)-	3	2
101,64	C10H14O2	1948-33-0	t-Butylhydroquinone	5	3
76,43	C12H4Cl6	52663-72-6	1,1'-Biphenyl, 2,3',4,4',5,5'-hexachloro-	2	2
55,96	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
51,44	C15H13N	2286-54-6	Benzenepropanenitrile, á-phenyl-	1	2
51,30	C12H5Cl5	52663-62-4	1,1'-Biphenyl, 2,2',3,3',4'-pentachloro-	1	2
45,74	C12H5Cl5	32598-14-4	1,1'-Biphenyl, 2,3,3',4,4'-pentachloro-	2	2
40,41	C9H10O2	140-11-4	Acetic acid, phenylmethyl ester	3	2
37,94	C9H10O3	10139-84-1	2',4'-Dihydroxy-3'-methylacetophenone	5	2
37,34	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
34,58	C8H6O2	1074-12-0	Phenyglyoxal	5	2
27,84	C9H8O	4432-63-7	2-Phenylpropenal	4	2
21,60	C12H5Cl5	55215-17-3	1,1'-Biphenyl, 2,2',3,4,6-Pentachloro-	3	2
20,67	C12H3Cl7	35065-30-6	1,1'-Biphenyl, 2,2',3,3',4,4',5'-heptachloro-	2	2
19,98	C14H10	85-01-8	Phenanthrene	2	2
18,17	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
16,73	C12H12O5	5062-30-6	Phenacylidene diacetate	4	2
12,64	C9H8Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	5	2
11,36	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	5	2
10,79	C8H7NS2	615-22-5	Benzothiazole, 2-(methylthio)-	3	2
7,94	C8H10O	123-07-9	Phenol, 4-ethyl-	1	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H8Br2O	147217-71-8	2,4'-Dibromodiphenyl ether (PBDE#7)	4	2
Qualitative	-	-	Natural product, Br3Cl3, probably monoterpene	4	5
Qualitative	C12H5Cl5	31508-00-6	PCB-118	7	2
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H5Cl5	32598-14-4	PCB-105	5	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6'-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6'-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2
Qualitative	C12Cl10	2051-24-3	PCB-209	7	2
Qualitative	C12H4Br6O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
Qualitative	C ₁₅ H ₁₂ Br ₄ O ₂	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
		58-63-9	Inosine	2	3
		89-39-4	1,4-dimethoxy-2-nitrobenzene	1	3
		477-93-0	dimethoxanate	1	3
		692-04-6	acetyllysine	1	3
		26088-14-2	9,9-bis(4-hydroxyphenyl)fluorene	1	3
		6786-83-0	α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalene-1-methanol		
		186817-80-1	Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester, (2S)-		
		147-94-4	cytarabine	1	3
		93-83-4	N,N-bis(2-hydroxyethyl)oleamide	1	3
		81-24-3	taurocholic acid	2	3
		1478-61-1	hexafluoroBPA (bisfenol AF)	3	1
		13595-25-0	bisphenol M	3	1
		550-24-3	embelin	2	3
		123-08-0	4-hydroxybenzaldehyde	6	3
		60-32-2	aminocaproic acid	4	3

Table 30: Fish Greenland

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
3269,82	C14H26O2	544-64-9	Myristoleic acid	6	2
1625,97	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
1297,39	C7H5NS	272-16-2	1,2-Benzisothiazole	3	2
523,11	C16H34O3	3055-93-4	Diethylene glycol monododecyl ether	1	2
440,01	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
422,28	C24H38O4	-	Phthalic acid, di(2-propylpentyl) ester	3	2
326,24	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
231,72	C13H20O	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	4	2
173,87	C23H40O3	71041-49-1	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	6	2
164,00	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
151,92	C16H33NO	629-54-9	Hexadecanamide	4	2
144,94	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
142,85	C13H20O	79-77-6	trans- δ -Ionone	1	2
136,39	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	3	3
135,77	C7H6O2	65-85-0	Benzoic acid	7	2
118,04	C11H16O2	17092-92-1	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	3	2
100,13	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
100,10	C13H16	30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	3	2
62,84	C13H18	30316-36-0	Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	1	2
58,22	C7H5NOS	934-34-9	2(3H)-Benzothiazolone	3	3
51,28	C21H36O3	86879-46-1	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	6	2
47,47	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
32,00	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
23,31	C8H6O2	1074-12-0	Phenylglyoxal	5	2
19,72	C9H18Cl3O4P	13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	5	2
18,59	C9H10O2	70-70-2	Paroxypropione	5	2
14,44	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
10,50	C9H8O	4432-63-7	2-Phenylpropenal	4	2
7,37	C9H12O2	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	4	2
3,97	C17H34O	55019-46-0	Hexadecanal, 2-methyl-	3	2
2,87	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H8Br2O	147217-71-8	2,4'-Dibromodiphenyl ether (PBDE#7)	4	2
Qualitative	C12H5Cl5	31508-00-6	PCB-118	7	2
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2
Qualitative	C12Cl10	2051-24-3	PCB-209	7	2
Qualitative	C12H4Br6O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C15H12Br4O2	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	1	3
	C18H26O3	5466-77-3	Ethylhexyl methoxycinnamate	1	3
	C11H18O4	90474-13-8	diethyl 1,2-cyclopentanedicarboxylate	1	3
	C10H14O3	59-47-2	mephensin	1	3
	C20H28O3	302-97-6	3-oxoandroster-4-ene-17 β -carboxylic acid	1	3
	C8H14O3	106-31-0	butyric anhydride	1	3
	C14H16ClN3O	67129-08-2	2-chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-yl)methyl acetamide		
	C13H17NO4	1086384-49-7	N-(2,6-dimethyl-phenyl)-N-(2-methoxy-ethyl)-oxalamic acid		
	C9H16O2	5726-19-2	2-methylcyclohexyl acetate	1	3

Continued

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
	C ₁₂ H ₁₅ N ₅ O ₅	75128-73-3	2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl)methoxy]ethyl acetate		
	C ₉ H ₇ NO	148-24-3	quinolin-8-ol	1	
		80-09-1	bisphenol S	2	1
		1478-61-1	hexafluoroBPA (bisfenol AF)	3	1
		843-55-0	bisfenol Z	3	1
		13595-25-0	bisphenol M	3	1
		1074-86-8	4-formyl indole	6	3
		60-32-2	aminocaproic acid	4	3
		584-44-1	Thymotic acid	2	3

Table 31: Fish Faroe Island

Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
1847,23	C17H36O2Si	18603-17-3	Tetradecanoic acid, trimethylsilyl ester	7	2
327,18	C10H16	3760-14-3	1,5-Cyclooctadiene, 1,5-dimethyl-	3	3
322,62	C7H5NS	95-16-9	Benzothiazole	5	2
320,67	C24H38O4	-	Phthalic acid, di(6-methylhept-2-yl) ester	2	2
268,32	C11H18O4	-	Fumaric acid, ethyl 3-methylbut-2-yl ester	7	2
163,14	C8H12O	30086-02-3	3,5-Octadien-2-one, (E,E)-	7	2
161,67	C17H25NO4	-	Succinic acid, 2-(dimethylamino)ethyl 4-isopropylphenyl ester	5	2
151,05	C9H10O2	70-70-2	Paroxypropione	5	2
142,27	C19H40O2Si	55520-89-3	Hexadecanoic acid, trimethylsilyl ester	7	2
115,22	C18H30	2719-62-2	Benzene, (1-pentylheptyl)-	2	2
111,15	C18H38O2Si	74367-22-9	n-Pentadecanoic acid, trimethylsilyl ester	6	2
109,28	C18H26O	1222-05-5	Galaxolide	4	2
94,00	C11H20	2958-76-1	Naphthalene, decahydro-2-methyl-	2	2
90,03	C7H6O2	65-85-0	Benzoic acid	7	2
82,76	C12H6Cl4	35693-99-3	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	7	3
67,36	C10H14O2	1948-33-0	t-Butylhydroquinone	5	3
62,81	C15H28	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	2	3
52,76	C12H24O3	74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	7	2
47,90	C17H28	4537-15-9	Benzene, (1-butylheptyl)-	2	2
43,62	C8H10N4O2	58-08-2	Caffeine	1	3
40,07	C7H5NS	272-16-2	1,2-Benzisothiazole	3	2
37,14	C14H10	85-01-8	Phenanthrene	2	2
33,89	C11H20	-	trans-Decalin, 2-methyl-	2	2
33,14	C12H22	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	2	3
33,07	C8H16O	5715-23-1	3,4-Dimethylcyclohexanol	6	2
26,09	C5H9NO2	4394-85-8	N-Formylmorpholine	7	2
25,97	C15H24	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	3	2
23,82	C12H22	66660-41-1	2-Ethyldecahydronaphthalene, (Z,E)-	2	2
12,25	C15H22O3	-	Salicylic acid, butyl ether, butyl ester	5	2
8,91	C17H34O	55019-46-0	Hexadecanal, 2-methyl-	3	2
Qualitative	C6H4Br2O	615-58-7	2,4-dibromophenol	7	2
Qualitative	C7H5Br3	607-99-8	2,4,6-tribromoanisole	7	2
Qualitative	C6H3Br3O	118-79-6	2,4,6-Tribromophenol	7	2
Qualitative	C12H8Br2O	147217-71-8	2,4'-Dibromodiphenyl ether (PBDE#7)	4	2
Qualitative	-	-	Natural product, Br3Cl3, probably monoterpene	4	5
Qualitative	C12H4Cl6	35065-27-1	PCB-153	7	2
Qualitative	C12H4Cl6	35065-28-2	PCB-138	7	2
Qualitative	C12H4Cl6	52663-72-6	PCB-167	7	2
Qualitative	C12H4Cl6	38380-08-4	PCB-156	7	2
Qualitative	C12H4Cl6	69782-90-7	PCB-157	7	2
Qualitative	C12H3Cl7	35065-29-3	PCB-180	7	2
Qualitative	C12H6Br4O	189084-61-5	2,3',4',6-Tetrabromodiphenyl ether (PBDE#47)	7	2
Qualitative	C12H3Cl7	35065-30-6	PCB-170	7	2
Qualitative	C12H3Cl7	39635-31-9	PCB-189	7	2
Qualitative	C12H5Br5O	93703-48-1	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE#100)	7	2
Qualitative	C12H2Cl8	52663-78-2	PCB-195	7	3
Qualitative	C12H2Cl8	35694-08-7	PCB-194	7	2
Qualitative	C12H5Br5O	60348-60-9	2,2',4,4',6-Pentabromodiphenyl ether (PBDE#99)	7	2
Qualitative	C12HCl9	40186-72-9	PCB-206	7	2
Qualitative	C12Cl10	2051-24-3	PCB-209	7	2
Qualitative	C12H4Br6O	68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE#154)	7	2
Qualitative	C15H12Br4O2	79-94-7	Tetrabromobisphenol A (TBBP-A)	7	2
		976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	1	3
		23680-84-4	2-chloro-6,7-dimethoxyquinazolin-4-amine	1	3
		14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	1	3
		363-24-6	dinoprostone	1	3
		108-59-8	dimethyl malonate	1	3
		34434-80-5	Abiet-8(14)-en-18-oic acid	2	3
		61443-78-5	Amoxapine-8-hydroxy	1	3
		26856-96-2	nonyl hydrogen sulfate	1	3
		80-09-1	bisphenol S	2	1

Continued					
Conc (ng/g)	Molecular Formula	CAS	Common name	Occur/ matrix	ID Level
		843-55-0	bisfenol Z	3	1
		13595-25-0	bisphenol M	3	1
		99-96-7	4-hydroxybenzoic acid	1	3
		123-08-0	4-hydroxybenzaldehyde	6	3
		1074-86-8	4-formyl indole	6	3
		584-44-1	Thymotic acid	2	3

Nordic Council of Ministers
Nordens Hus
Ved Stranden 18
DK-1061 Copenhagen K
www.norden.org

SUSPECT SCREENING IN NORDIC COUNTRIES

This report describes the results of a suspect screening study in samples from city areas in the Nordic countries. In contrast to target analysis, suspect screening starts with a general sample preparation and identification including as much compounds as possible. The resulting list of recorded compounds will be identified by comparison with a list of suspected compounds. Suspect screening has shown to be very useful for identification of emerging environmental pollutants. It was possible to identify: Perfluorinated compounds (PFC), chlorinated and brominated compounds, flame retardants, bisphenols, polycyclic aromatic compounds (PAC), industrial additives, and pharmaceuticals and personal care products (PPCP). This study was jointly performed by NILU, NIVA, and Umeå University on behalf of the Nordic Council of Ministers. The study was supervised by the Nordic screening group.

9 789289 351997