MILJØ-DIREKTORATET

Norsk institutt for vannforskning

NILU

ENVIRONMENTAL MONITORING

M-446 | 2015

Screening program 2014

Organic phosphites, selected PBT substances and non-target screening

COLOPHON

Executive institution

Norsk institutt for vannforskning (NIVA) and
NILU - Norsk institutt for luftforskning

ISBN-no

978-82-577-6663-4

Project manager for the contractor

Kevin Thomas & Martin Schlabach

Contact person in the Norwegian Environment Agency

Eivind Farmen

M-no	NIVA-no	NILU-no	Year	Pages	Contract number
446	6928-2015	OR33/2015	2015	148	14078113

Publisher

Norwegian Environment Agency

The project is funded by

Norwegian Environment Agency

Author(s)

Kevin Thomas (NIVA), Martin Schlabach (NILU), Kathrine Langford (NIVA), Malcolm Reid (NIVA) Eirik Fjeld (NIVA), Sigurd Øxnevad (NIVA), Thomas Rundberget (NIVA), Kine Bæk (NIVA), Pawel Rostkowski (NILU), Laura Röhler (NILU/NMBU) and Anders Borgen (NILU)

Title - Norwegian and English

Screening programme 2014: Phosphites, selected PBT substances and non-target screening
Screening program 2014: Fosfitter, utvalgte PBT stoffer og hypotesefri miljøscreening

Summary - sammendrag

The occurrence and environmental risk of a number of phosphites and selected PBT substances are reported for wastewater effluents and leachates, as well as sediments and biota from Oslofjord and Lake Mjøsa. In addition a suspect and non-target screening approach was applied to approximatley half of the biota samples.

Forekomsten og miljørisiko av en rekke nye fosfitter og utvalgte PBT stoffer er rapportert for utslipp fra avløpsrenseanlegg og sigevann, samt sedimenter og biota fra Oslofjorden og Mjøsa. I tillegg ble det utført en hypotesefri miljøscreening av halvparten av alle biotaprøver.

4 emneord

Nye miljøgifter, hypotesefri miljøscreening, forekomst, næringskjeden

4 subject words

Emerging contaminants, non-target screening, occurrence, food chain

Front page photo

Oslofjord (Shutterstock Inc.)

Summary

Upon assignment from the Norwegian Environment Agency (Miljødirektoratet), the Norwegian Institute for Water Research (NIVA) and Norwegian Institute for Air Research (NILU) have together performed a screening of organic phosphites and selected PBT (persistent, bioaccumulative and toxic) compounds in freshwater and marine environments. Organic phosphites are typically high production volume chemicals that are used as plastic additives, while the selected PBT compounds were 2,6-di-tert-butyl-p-cresol (BHT), 2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether (PBO), dibenzyltoluene, 6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol, octabenzone, tris(tribromoneopentyl) phosphate and 4,4'-methylenediphenyl diisocyanate. The objective of the project was to establish the occurrence of these chemicals in Norwegian marine and freshwater environments, with particular focus on their potential to bioaccumulate.

The most important findings can be summarized as follows:

Organic phosphites
None of the samples collected contained any of the organic phosphites selected for screening at concentrations above the limits of detection.

Selected PBT compounds
BHT and PBO were the only PBT substances detected in the study. Wastewater treatment works (WWTW) effluent is a source of BHT and PBO with concentrations of between <LoD and 1,200 ng/L and <LoD and 782 ng/L released into the environment respectively. WWTW sludge is a source of BHT with concentrations of between 98 and 812 ng/g. BHT was also present in landfill leachates (200 – 1,390 ng/L) and shown to accumulate in marine and freshwater sediments receiving treated wastewater (18-102 ng/g). BHT was found in biota from both Oslofjord and Lake Mjøsa. For example trout from Mjøsa contained between 7 and 25 ng/g and cod livers from Oslofjord between 0.5 and 12 ng/g. Similar levels were also detected in the livers of rats collected from Oslo (0.5-13 ng/g). A closer inspection of the BHT and PCB153 concentrations and of the isotopic ratios ($\delta^{15}N$ and $\delta^{13}C$) revealed that BHT did not bioaccumulate in the food chain, but rather showed sign of biodilution at higher trophic levels

Neither BHT nor PBO were present in WWTW effluent at concentrations above the PNECs for receiving waters and therefore pose little direct risk. There may be a risk associated with the accumulation of BHT in sediments and biota, however, this has not been evaluated.

Non-target screening
Suspect and non-target screening was applied to two aquatic food-chains, one from Lake Mjøsa and one from Oslofjord, as well as samples of rat collected from Oslo. Five compounds were identified in all levels of the Oslofjord foodchain studied; galaxolide, hexachlorobiphenyl, p,p´-DDE, PFOS and PFOSA. Tonalide and carbenoxolone were identified in all levels of the Oslofjord foodchain apart from cod. Nine compounds were identified in all studied trophic levels of the Lake Mjøsa foodchain studied; 1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one, hexachlorobiphenyl, stearic acid monoester with glycerol, buprenorphine, 1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethylnaphthalen-2yl]ethan-

1-one (OTNE), dodecylphenol, p,p'-DDE, p,p'-DDT, nitrophenylhydrazine. A further two compounds, 4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone, 3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone, were found in all levels of the foodchain apart from brown trout. In rats, benzophenone was the only compound identified at the highest level of certainty (level 1), with diethyl phthalate, dibutyl phthalate, methyl hexadecyl ketone, isopropyl palmitate, elaidic acid, isopropyl ester, pentachlorobiphenyl, isopropyl stearate, octadecanoic acid, butyl ester and butyl myrisate tenatativley identified (evel 2).

Non-target and suspect screening generates a large amount of potentially useful information. However, existing technology for processing, filtering and prioritizing of the findings make this task extremely time consuming with existing instrument software/hardware combinations at their limit of applicability. A significant observation from this project was the difficulty in separating naturally occurring compounds from those of anthropogenic origin, with a need to investigate the 1000´s of naturally occurring compounds manually on an individual basis. To further develop the full capabilities of non-target screening there is a need to improve the software-hardware combinations that are currently used for data evaluation.

Sammendrag

På vegne av Miljødirektoratet har NIVA - Norsk institutt for vannforskning og NILU - Norsk institutt for luftforskning, i fellesskap gjennomført en screeningstudie av organiske fosfitter og utvalgte PBT (persistente, bioakkumulerende og giftige) forbindelser i et marint og et ferskvannsmiljø. Organiske fosfitter er kjemikalier som vanligvis produseres i store kvanta og benyttes som plastadditiver. De utvalgte PBT forbindelsene er 2,6-di-tert-butyl-p-kresol (BHT), 2-(2-butoksyetoksy)etyl-6-propyl-piperonyl eter (PBO), dibenzyltoluen, 6,6'-di-tert-butyl-2,2'-metylen-p-kresol, octabenzone, tris(tribromoneopentyl)fosfat og 4,4'-metylendifenyldiisocyanat. Målet med prosjektet var å undersøke forekomsten av disse kjemikaliene i norske marine og ferskvannsmiljøer, med særlig fokus på deres potensiale for bioakkumulering.De viktigste resultater kan oppsummeres som følger:

Organiske fosfitter
Ingen av de innsamlete prøvene inneholdt noen av de valgte organiske fosfitter i konsentrasjoner over deteksjonsgrensen.

Utvalgte PBT forbindelser
Av de valgte PBT-stoffene var det kun BHT og PBO som kunne detekteres. Avløpsvann fra renseanlegg er en kilde til BHT og PBO og utslippskonsentrasjoner ligger henholdsvis mellom <LoD og 1 200 ng/L og <LoD og 782 ng/L. Slam fra renseanlegg er en kilde til BHT og slamkonsentrasjoner mellom 98 og 812 ng/g tørrvekt er blitt målt. BHT var også til stede i avrenning fra fyllinger (200 – 1 390 ng/L) og marine- og ferskvannssedimenter som mottar renset avløpsvann viser BHT-konsentrasjoner mellom 18 og 102 ng/g tørrvekt. BHT ble også påvist i biota fra både Oslofjorden og Mjøsa. For eksempel inneholder ørret fra Mjøsa mellom 7 og 25 ng/g og torskelever fra Oslofjord mellom 0,5 og 12 ng/g. Lignende nivåer ble også påvist i rottelever som var samlet inn fra Oslo (0,5 til 13 ng/g). En sammenligning av BHT- og PCB-153 konsentrasjonene med isotop ratioene ($\delta^{15}N$ og $\delta^{13}C$) avdekker at BHT ikke bioakkumulerer i næringskjeden, men at stoffet heller viser tegn for biofortynning oppover i næringskjeden.

Verken BHT eller PBO i avløpsvann ble detektert i konsentrasjoner over de eksisterende PNEC verdiene for resipienten og utgjør derfor liten direkte fare. Det kan være en risiko forbundet med opphopning av BHT i sedimenter og biota, men dette er ikke vurdert.

Hypotesefri miljøscreening
Forskjellige former av hyposefri miljøscreening («suspect» og «non-target» screening) ble gjennomført for utvalgte prøver fra to akvatiske næringskjeder (Oslofjord og Mjøsa) samt for fem prøver av rotter fra Oslo. I næringskjeden fra Oslofjord var det mulig å påvise og identifisere fem forskjellige stoffer i alle nivåer av næringskjeden: galaxolid, hexachlorobiphenyl, p,p´-DDE, PFOS og PFOSA. Tonalid og carbenoksolon kunne påvises i alle nivåer av næringskjeden untatt torsk. I næringskjeden fra Mjøsa var det mulig å påvise og identifisere ni forskjellige stoffer: 1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-sykloheksen-1-yl]ethan-1-on, heksaklorobifenyl, stearinsyremonoester med glycerol, buprenorfin, 1,2,3,4,5,6,7,8-oktahydro-2,3,8,8-tetrametylnaftalen-2yl]etan-1-one (OTNE), dodecylfenol, p,p'-DDE, p,p'-DDT og nitrofenylhydrazin. To andre stoffer, 4-(5,5,6-trimetylbisyklo[2.2.1]hept-2-yl)sykloheksanon og 3-(5,5,6-Trimetylbisyklo[2.2.1]hept-2-

yl)sykloheksanon ble identifisert i alle nivåer unntatt ørret. I rotter ble benzofenon identifisert med høyest grad av sikkerhet (dvs. identifikasjonsnivå 1) og dietylftalat, dibutylftalat, metylheksadekylketon, isopropylpalmitat, elaidinsyreisopropylester, pentaklorobifenyl, isopropylstearat, octadekanonsyrebutylester og butylmyrisate ble identifisert tentativ, det vil si med identifikasjonsnivå 2.

Hypotesefri miljøscreening generer en stor mengde potensiell verdifull informasjon. Per i dag er den tilgjengelige teknologien for dataprosessering, filtrering og prioritering av alle funnene ikke tilstrekkelig utviklet slik at denne jobben er ekstremt tidkrevende. En annen viktig observasjon er at det vanskelig å skille naturlig forekommende stoffer fra stoffer av antropogen opprinnelse. Her var det nødvendig å fjerne tusenvis av naturlige forkommende stoffer manuelt. For å kunne utnytte det fulle potensiale av hypotesefri miljøscreening er det nødvendig å tilpasse og optimalisere software-hardware kombinasjonen som brukes til databehandlingen.

Contents

1. Background and Introduction

1.1 General

The Norwegian Environment Agency in 2014 selected two groups of compounds for target analysis for inclusion in Part 1 of its annual screening programme. These were organic phosphites and seven selected PBT compounds. The objective of the project was to establish the occurrence of these chemicals in the Norwegian marine and freshwater environments, with particular focus on their potential to bioaccumulate. In Part 2 of the project non-target analytical methods were used to identify as many compounds as possible present in a marine and freshwater foodchain.

1.2 Organic phosphites

Organic phosphites are a diverse group of chemicals, all of which are typically used in industrial processing and the manufacturing of plastics. They are typically used as additives to improve stability, often as antioxidants. No previous surveys on the occurrence of organic phosphites have been reported and subsequently very little is known about their environmental occurrence, even though the vast majority are high production volume chemicals with annual production of between a 100 and 100,000 tonnes.

Tris(nonylphenyl)phosphite (TNPP) is used in industrial processing, other plastic product manufacturing and plastic packaging materials, unlaminated film, and sheet manufacturing as a stabilizer; resin and synthetic rubber manufacturing as well as tire manufacturing. Available data on the use of TNPP in the Nordic countries suggest that in excess of 500 tonnes is used annually. Should TNPP be released into an aqueous compartment then it will hydrolyse to form nonylphenol, a known endocrine disrupter, however, laboratory hydrolysis studies suggest that the level of hydrolysis in water is low and that it is not an important transformation pathway. TNPP is also considered not biodegradable in aquatic environments. TNPP may be released into the environment following production, transport, storage, formulation, the processing, use and disposal of plastic and rubber products (EU, 2002). **Isodecyl diphenyl phosphite (DPDP)** is also used in plastic manufacturing. DPDP is assumed to be rapidly hydrolysed in water based upon the half-life of 0.5 h for **triphenyl phosphite (TPPi)**. **3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane** (Irgafos 162) is poorly soluble in water and has also been shown to rapidly hydrolyse. **Triisodecyl phosphite** (TDP) is also hydrolytically unstable with a half-life of 17 h at pH 7 (23 °C), while **triisotridecyl phosphite** has a hydrolysis half-life of 0.43 h. **Tris(2,4-ditert-butylphenyl) phosphite** is however hydrolytically stable and shows little susceptibility to biodegradation under laboratory conditions. **Tetrakis(tritolyl phosphite)nickel** (TTP) is reported to be essentially insoluble in water and undergo hydrolysis when exposed to an aqueous solution. In summary, organic phosphites are a group of high production volume chemicals that are highly hydrophobic and in most cases rapidly hydrolyse in contact with water.

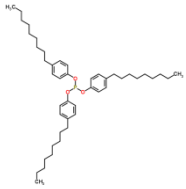
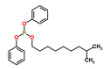
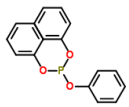
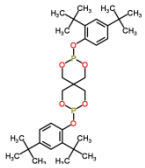
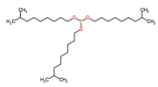
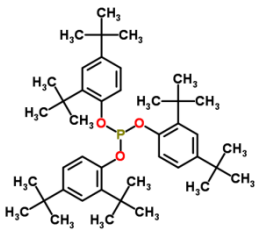
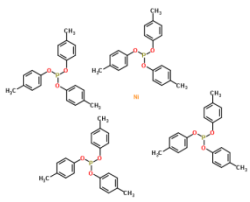
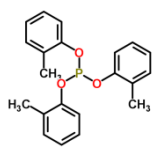
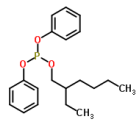
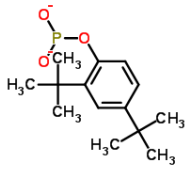
Table 1: Organic phosphites selected for screening					
Compound	**Acronym**	**Structure**	**CAS**	**Function**	**Log K_{OW}**
Tris(nonylphenyl)phosphite	TNPP		26523-78-4	Plastic additive	20[†]
Isodecyl diphenyl phosphite	DPDP		26544-23-0	Plastic additive	5.52[†]
Triphenyl phosphite	TPPi		101-02-0	Plastic additive	6.6[†]
3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane	Irgafos 126		26741-53-7	Plastic additive	10.9[†]
Triisodecyl phosphite	TDP		25448-25-3	Plastic additive	12.3[†]
Triisotridecyl phosphite	TiTDP		77745-66-5	Plastic additive	16.7†
Tris(2,4-ditert-butylphenyl) phosphite			31570-04-4	Plastic additive	18.1[†]
Tetrakis(tritolyl phosphite)nickel	TTP		35884-66-3	Plastic additive	7
Tris(methylphenyl)phosphite			25586-42-9	Plastic additive	7[‡]

Table 1: Organic phosphites selected for screening					
Compound	**Acronym**	**Structure**	**CAS**	**Function**	**Log K_{OW}**
Diisodecyl phenyl phosphite	PDDP		25550-98-5	Plastic additive	9.32†
2-Ethylhexyl diphenyl phosphite			15647-08-2	Plastic additive	7.54†
O,O'-dioctadecylpentaerythritol bis(phosphite)	Irgafos 168		3806-34-6	Plastic additive	16.4†

† QSAR predicitons; ‡ Read-across from TPP.

1.3 Selected PBT and other compounds

The group of selected PBT and other compounds are very diverse and consist of both additives as antioxidants, a UV-stabilizer, and flame-retardants on one hand and a heat transfer fluid and a monomer on the other hand (Table 2).

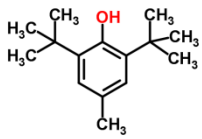
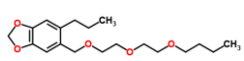
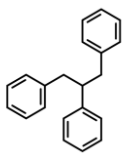
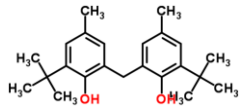
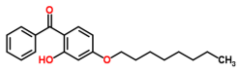
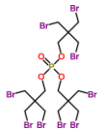
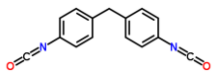
Table 2: PBT and other compounds selected for screening					
Compound	**Acronym**	**Structure**	**CAS**	**Function**	**Log K_{OW}**
2,6-di-tert-butyl-p-cresol	BHT		128-37-0	Antioxidant	5.32
2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether **(Butocide)**	PBO		51-03-6	Synergist in pesticide formulations	4.23
Dibenzyltoluene	DBT	 And other isomers	26898-17-9	Heat transfer fluid	6.49

Table 2: PBT and other compounds selected for screening					
Compound	**Acronym**	**Structure**	**CAS**	**Function**	**Log K_{OW}**
6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	AO2246		119-47-1	Antioxidant	7.03
Octabenzone	Octabenzone		1843-05-6	UV filter	7.36
Tris(tribromoneopentyl) phosphate	TTBPP		19186-97-1	FR	9.03
4,4'-methylenediphenyl diisocyanate	MDI		101-68-8	Plast monomer	4.93

In 2000, the world production capacity for **2,6-di-tert-butyl-p-cresol (BHT)** was 62,000 tonnes per annum by more than 20 producers. BHT is a registered antioxidant, licenced for food products, animal feed, cosmetics, and packaging material. It is also used in petroleum products, synthetic rubbers, plastics, elastomers, oils, waxes, soaps, paints, and inks. Releases into the environment may occur during production of BHT as well as during its use in different applications as a stabilizer and during the use of the products that contain the substance. A significant release into the environment is expected from the migration of BHT onto the surface of products containing the substance. Most organic materials undergo oxidation reactions and the most commonly used protection protocol is the addition of antioxidants, in which synthetic phenolic antioxidants (SPAs) are the most frequently used. Toxicity studies showed that the metabolites of BHT, such as 3,5-di-tert-butyl-4-hydroxybenzaldehyde (BHT-CHO), 2,6-di-tert-butyl-1,4-benzoquinone (BHT-Q) and 2,6-di-t-butyl-4-hydroxy-4-methyl-2,5-cyclohexadienone (BHT-quinol), could generate peroxides in mice and rats and induce cellular DNA damage (Liu et al., 2015).

2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether (PBO) is mainly used as a synergist in pesticide formulations, typically insecticides, such as pyrethroids or natural pyrethrins. As a synergist, PBO works by inhibiting the detoxification of the pesticide by the insects. As it is used in modern pesticide formulations, it is frequently found in fruits and vegetables.

Dibenzyltoluene (DBT) is used as a dielectric and heat transfer fluid in closed systems. Technical DBT is a mixture of several structural isomers. DBT was found in leachate samples from some production related hazardous waste dump sites close to Niagara falls, USA in the 1980s (Elder et al., 1981).

6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol (AO 2246) is also a synthetic phenolic antioxidants (SPAs) which is mainly used to prevent ageing of natural rubber, synthetic rubber and synthetic resin. It was found to be a direct testicular toxin in rats (Liu et al., 2015).

Octabenzone (Spectra-Sorb UV 531, MPI Milestab 81) is a UV absorber/screen. It is used to protect polymers (e.g., polyethylene, polypropylene, polyvinylchloride) against damage by UV light.

Tris(tribromoneopentyl) phosphate (TTBNPP) is marked as a replacement for HBCD in the flame proofing of extruded polystyrene (XPS) (Managaki et al., 2011). A recent theoretical evaluation of the overall persistence and long-range transport potential of new brominated flame retardants calculated a life time in water for of much more than 2 months, hence, characterizing this compound as very persistent in the environment (Kuramochi et al., 2014). In an EFSA modelling exercise tris(tribromoneopentyl) phosphate (TTBNPP) was predicted as likely to have a high persistence, but likely to rapidly undergo metabolic breakdown in vivo, and thus not be bioaccumulative (Benford et al., 2012).

4,4'-methylenediphenyl diisocyanate (MDI) is an important monomer for polyurethane (PUR) production. The diisocyanate monomers are very reactive chemicals, but known as respiratory sensitizers and cause irritation of eyes, skin and mucous membrane. When MDI is added to water, its NCO groups react readily with OH groups of the water to form mixtures of diisocyanates and amines, which then readily react with more MDI to produce inert, solid, insoluble polyurea. The hydrolysis of isocyanates in aqueous solution is rapid; a half-life of 20 s has been measured for phenyl isocyanate. However, the subsequent reaction of the formed amine with further isocyanate, to produce a urea, is even faster (Sekizawa and Greenberg, 2001).

1.4 Non-target and suspect screening

Conventional chemical analysis, as described above for phosphites and selected PBT and other compounds, targets a specific compound or group of compounds and as such is termed **target analysis** (Figure 1). Target analysis involves optimizing the conditions of an analytical method to a specific target analyte or group of analytes with similar chemical properties. This is to say that all steps of the analytical workflow, extraction, chromatographic separation and detection are all optimized to provide a specific and accurate measurement. Target analytical methods are typically quantitative, a feature that is often facilitated by using isotopically labeled internal standards that are analogues of the target analytes. Over the past few years analytical instrumentation has also evolved to allow additional screening of environmental samples using a 'non-target' approach in an attempt to identify the compounds present in an environmental sample. The main instrumental advancement that has facilitated the development of non-target analysis is the evolution of accurate mass high-resolution mass spectrometry (HRMS). Non-target and suspect screening using HRMS complement targeted analysis as shown in Figure 1. Similarly to target analysis, **suspect screening** uses prior knowledge to search for the presence of a substance in a sample, however without the use of a reference standard. 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 inform the suspect screening process, such as those sold by instrument producers and those in the public domain, such as STOFF-IDENT, MassBank or ChemSpider. An effective suspect list for environmental screening is essentially a prioritized list of compounds that one would expect to find in the environment, along 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 that is freely available (http://www.norman-network.com/?q=node/236).

Non-target screening involves the identification of peaks in the chromatogram that are unknown and about which no prior knowledge 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 the different identification approaches versus the confidence in identification (Figure 1). Level 1 equates to the level of confidence from conventional target analysis, where an authentic reference standard is available and 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 insufficient information for only one exact structure. Level 4 describes the unequivocal molecular formula and level 5 the exact mass of interest. For this purpose of this report only compounds identified with a confidence of level 3 or above are reported.

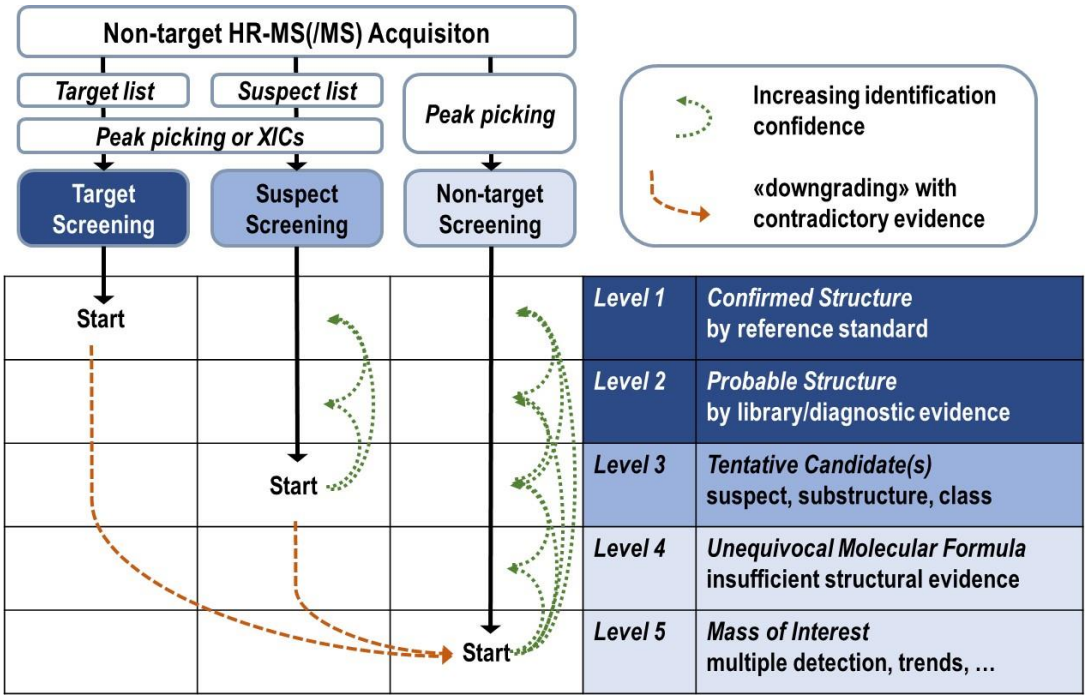


Figure 1: Matrix showing the identification approach versus confidence of confirmation. Copied with permission from Schymanski et al. 2015.

2. Materials and Methods

2.1 Sample Collection

2.1.1 Wastewater treatment works

All of the wastewater treatment works (WWTW) samples were collected by staff at the respective plants. They were kindly asked not to use plastic gloves during sampling and to avoid the use of personal care products. Twenty four hour composite effluent samples were collected by means of the automatic sampling equipment already found at the WWTWs for routine monitoring. The effluent samples were collected in clean glass bottles and shipped to NIVA. Sludge samples were collected using a procedure based on the Mattilsynet guideline for the sampling of sludge, compost and other waste-based fertilizer products. Five core samples of mixed sludge were collected from each facility. Each mixed sample was transferred to 4 glass sample jars using pre-washed stainless steel equipment provided by NIVA.

• Vestfjorden avløpsselskap (VEAS) at Slemmestad is Norway´s largest WWTW receiving municipal wastewater from a population of around 550,000. The plant annually receives between 100-110 million m^3 of wastewater that is treated mechanically, chemically and biologically (post-denitrification). The sludge is treated by anaerobic digestion and drying. The treated effluent is discharged at a depth of approx. 50 m depth in the Oslofjord .

• HIAS owned and receives wastewater from approximatley 52,000 people from the municipalities of Hamar, Løten, Ringsaker, and Stange. The plant is located at Ottestad on Lake Mjøsa with the discharge point at a depth of 15 m around 250 m from the shore. Wastewater is treated mechanically, biologically (not N removal) and chemically. The sludge is treated by thermal hydrolysis (Cambiprocess at 160 °C) prior to anaerobic digestion at 38°C.

• Tomasjord WWTP in the municipality of Tromsø is a primary WWTP with a capacity of 38,400 person equivalents. The wastewater is primarily domestic sewage and the mechanical treated wastewater is discharged into Tromsøysundet.

2.1.2 Landfill sites

Leachate sampling was performed using an ISCO 6712 automatic sampler for collecting a 24 hr composite sample from ISI landfill and Lindum Resource and Recycling AS. Flow data were obtained from the plants own water flow measurements.

• ISI landfill (Bærum Kommune) was established in 1974 and ceased being used in 2002. ISI covers an area of approximately 1.4 km^2 with a fill depth of between 12 and 21 m. Groundwater levels in the landfill can be 7.2 m above the base of the landfill. The draining water, composed of leachate and incoming groundwater, flows through a discharge tank downstream of the landfill. Leachate from ISI is sent to VEAS WWTW for treatment.

• Lindum Resource and Recycling is located in Drammen and receives solid waste from the Drammen Region. Leachate from the landfill is heavily influenced by incoming groundwater, especially in the wake of heavy rainfall events. The total annual leachate volume in the

period 2000-2006 was at 366,000 to 910,000 m^3. All the leachate goes through an aerated lagoon with subsequent sedimentation before it is pumped to Solumstranda WWTW.

2.1.3 Inner Oslofjord

Sediment

Sediment samples were collected at five stations along a transect from close to the discharge diffuser from the VEAS WWTW and southward in the deep-water channel of Oslofjord (Figure 2). On the west side of the fjord, the tidal current runs in a southerly direction and is split by a vortex near the middle of the fjord south of Søndre Langåra. There are also currents through Ristsundet on the east side of Håøya, and one current on the west side of Håøya (Gråøyrenna). On rising tide most of the current flows on the east side of Håøya. Sediment stations were placed in the deep channel on both sides of Håøya. The sediment stations were on approximately same depths. Sediment was collected with a stainless steel Van Veen grab (Picture 1). Four replicate samples of the top 2 cm of the sediment were collected from each station. Each sample was a mixed composite from three grabs.

Figure 2. Map of the sediment stations in the Oslofjord.

Picture 1: Sediment was collected from five stations with a Van Veen grab (photos: Sigurd Øxnevad, NIVA).

Atlantic cod and herring

Atlantic cod (*Gadus morhua*) and herring (*Clupea harengus*) were caught by trawling from the research vessel F/F Trygve Braarud during August 2014 (Picture 2). The cod were caught in the area between Askerlandet and Steilene in the Inner Oslofjord and ranged in size from 0.753 to 6.9 kg (Table 3). Individual samples of liver were removed for chemical analysis and stored in heat-treated (500 °C) glass containers sealed with heat-treated aluminium foil underneath the lids. Samples were stored frozen (-20 °C) until analysis.

Picture 2: Samples of cod from the Inner Oslofjord (photos: Sigurd Øxnevad, NIVA).

Table 3: Size, sex and liver weight of cod caught in the Inner Oslofjord				
Fish No.	Length (cm)	Weight (kg)	Sex (M/F)	liver weight (g)
1	54	1.414	F	34
2	47	1.232	F	43
3	42	0.759	M	26.4
4	41	0.753	F	22.5
5	49	0.976	F	21.5
6	51	1.171	M	39
7	50	1.101	F	16.5
8	70	3.540	F	122
9	71	4.600	F	74
10	78	6.930	F	165

Northern shrimp and krill

Northern shrimp (*Pandalus borealis*) and krill were caught by trawling from the research vessel F/F Trygve Braarud during August 2014 (Picture 3). The shrimps were peeled and split into 15 bulk samples. Each sample was comprised of between 50 and 60 individual shrimps.

Picture 3: Northern shrimp and krill were caught by trawling in the Inner Oslofjord (photos: Sigurd Øxnevad, NIVA).

2.1.4 Lake Mjøsa

Sediment

Five pooled samples of sediment were taken along a gradient from the discharge point to HIAS and south (Table 4). Each pooled sample consisted of three individual subsamples taken from the upper 0-2 cm sediment layer at a water depth of 25–35 m. We used a gravity corer with a core tube and a retractable sediment stopper in stainless steel. The samples were transferred to heat-treated (500 °C) glass containers sealed with heat-treated aluminium foil underneath the lids. The core tube and other sectioning equipment used were thoroughly cleaned with acetone and cyclohexane (HPLC grade) before

use, and direct hand contact with the sampling matrix was avoided. They samples were stored frozen (-20 °C) until analysis.

Fish

From Lake Mjøsa, during August 2014, we collected the following species of pelagic fish: brown trout (*Salmo trutta*), smelt (*Osmerus eperlanus*) and vendace (*Coregonus albula*). Smelt and vendace were caught with gillnets, deployed in the area around the outlet of discharge pipe of the HIAS sewage treatment plant, at a depth of about 20 – 35 m, whereas brown trout were caught north of the town of Gjøvik at a depth of 5 –20 m (Table 4). The smelt belonged to two size groups: small bodied planktivorous individuals and somewhat larger cannibalistic individuals. 10 samples were prepared of each species and size group (smelt).

The fish were taken out of the nets as they were hauled, instantly killed with a short blow to the head, wrapped in clean aluminium foil, kept cool and transported to a freezer (-20 °C). Before freezing the aluminium foil wrapped fish were put in polyethylene bags. At no time were the fish allowed to be in contact with plastics or other potentially contaminated surfaces. The time between catch and transfer to the freezer took no longer than 4 hours.

Before preparing samples of the benthic fish, they were thawed, scraped clean of mucus with a solvent washed knife and placed on a cutting board covered with solvent rinsed aluminium foil. For each fish a solvent cleaned set of stainless steel dissection tools was used. We dissected the sagittal otoliths, and determined sex and maturity after opening of the abdomen. We dissected out samples of lateral skeleton muscles and transferred them to heat treated (500 °C) glass containers sealed with heat-treated aluminium foil underneath the lids. The samples were then frozen (-20 °C) and sent to homogenization before analysis. 10 individual samples were prepared of each species and size group (two groups of smelt). For the small bodied planktonivorous smelt we had to make pooled samples from about 3-5 individuals for each to obtain sufficient material for chemical analysis.

To reduce the risk of contamination during catch and sample preparation, all personnel involved avoided use of personal care products at least 24 hours in advance. Also, dissection and preparing of samples took place outside in a non-urban area. Dissection equipment and aluminium foil that could be in direct contact with the samples were cleaned with acetone and cyclohexane (HPLC grade) before use, and direct hand contact with the sampling matrix was avoided.

Mysis and zooplankton

Samples of the opossum shrimp *Mysis relicta* and zooplankton were sampled with horizontal net hauls. Epipelagic zooplankton, consisting mainly of the cladoceran *Daphnia galeata* and *Bosmina longispina*, were collected at a depth of 3–5 m, whereas hypopelagic Mysis and zooplankton (mainly the copepods *Limnocalanus macrurus*, *Cyclops lacustris* and *Eudiaptomus gracilis*) were collected at a depth of 70–110 m. The zooplankton net used were made of nylon mesh (single strand thread, mesh size: 500 µm), equipped with a brass cup with a brass mesh, and with an opening diameter of 1 m.

Mysis were separated from copepods in the epipelagic samples by filtering the samples through a sieve (mesh of stainless steel strands) while flushing gently with water from the lake and handpicking with tweezers. All filtering and separation of samples were done in the boat immediately after net hauling. The samples were kept on the same type of cleaned class jars as the fish, held cool on board until they could be transferred to a freezers (-20 °C) no more than 8 hours after sampling. All equipment (glass or metal) and aluminium foil that could be in direct contact with the samples after they were transferred

from the net were cleaned with acetone and cyclohexane (HPLC grade) before use, and direct hand contact with the samples was avoided. We prepared 10 samples of Mysis and 5 samples of epi- and hypopelagic zooplankton, respectively.

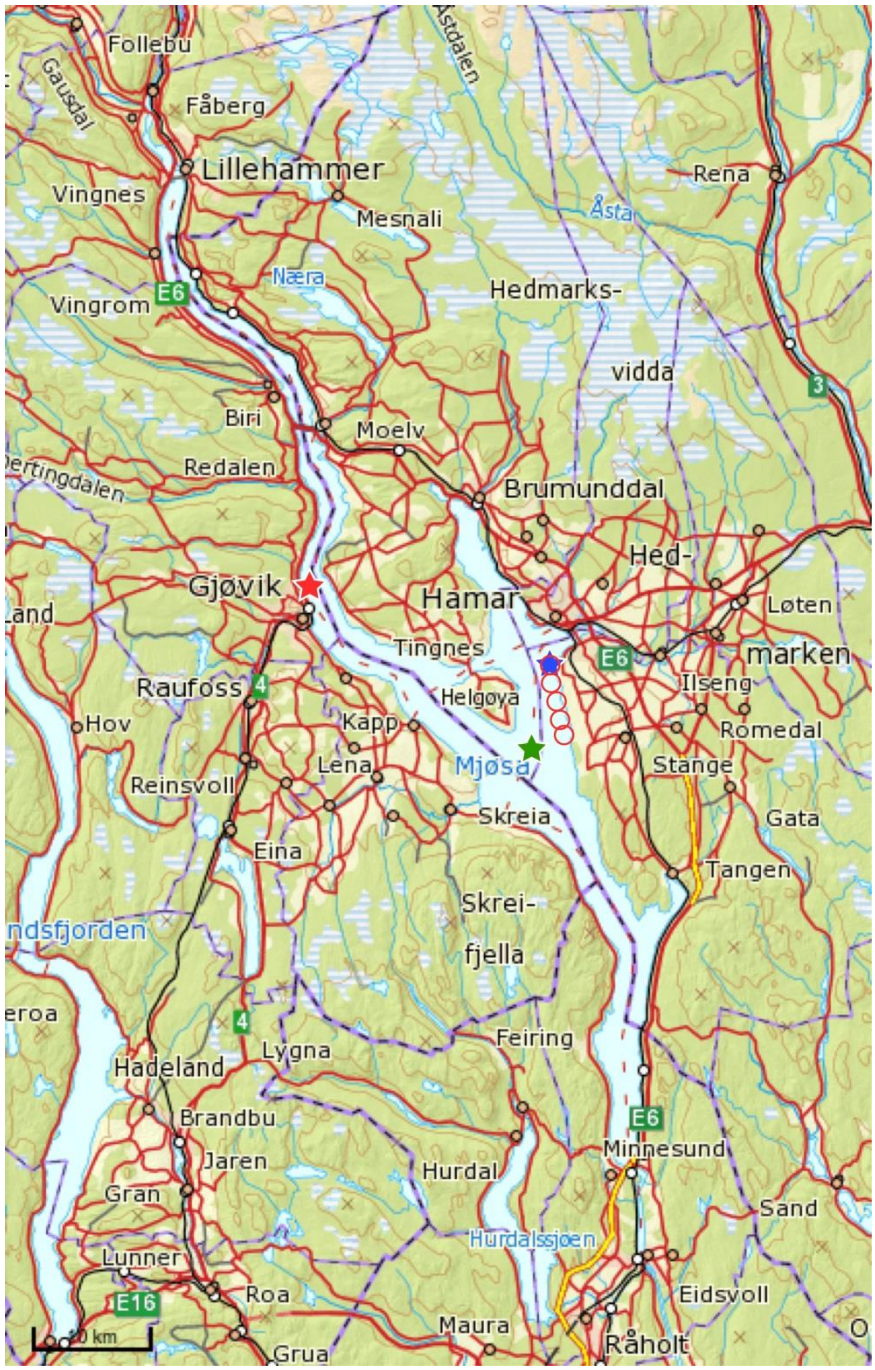


Figure 3: Map showing Lake Mjøsa, the catch sites (blue star: smelt and vendace; red star: brown trout; Mysis and zooplankton: green star) and sediment sampling sites (red circles). The location coordinates are given in Table 4.

Table 4: Coordinates for the Lake Mjøsa sediment and biota sampling stations						
Station	Date	Depth (m)	UTM 33E	UTM 33 N	°E	°N
Sediments						
St-1	18.08.13	35	286400	6743600	11.059	60.766
St-2	18.08.13	25	285941	6742150	11.075	60.759
St-3	18.08.13	25	285932	6740684	11.072	60.744
St-4	18.08.13	25	286479	6739302	11.084	60.732
St-5	18.08.13	25	287021	6737370	11.096	60.715
Fish						
St-1	15-30.08.14	20–35	286400	6743600	11.059	60.766
St. Gjøvik	15-30.08.14	10–20	265100	6750000	10.680	60.816
Mysis and zooplankton	15-30.08.14	epipelagic: 3–5 m hypopelagic: 70–110 m	284000	6735000	11.04	60.69

2.1.5 Rats

Rat samples were provided frozen by Anticimex (Picture 4). The rats were caught in a residential property in Oslo using traps and the livers removed for analysis.

Picture 4: The rats selected for analysis (photo: Sigurd Øxnevad, NIVA).

2.2 Chemical analysis

2.2.1 Organic phosphites

Reagents and standard solutions
Phosphites, CAS No.s 31570-04-4, 25448-25-3, 26523-78-4, 3806-34-6, 101-02-0 were purchased from Sigma-Aldrich. CAS No.s 26741-53-7 and 26544-23-0 were obtained from Chemos Gmbh and CAS no.s 15647-08-2, 77745-66-5 and 25550-98-5 were kindly provided by Akros Chemicals, UK. No commercially available standards were available for CAS No.s 35884-66-3 and 125586-42-9. For these two compounds an approach was used where the MS mass transitions were determined theoretically and samples were monitored for their occurrence. Based upon the confidence matrix presented in Figure 1 this would represent a level 3 identification, however no such peaks were observed.

Other reagents and solvents (methanol, acetonitrile, hexane, cyclohexane, formic acid and ammonium formate) were of HPLC or analytical-reagent grade and obtained from Rathburn Chemicals (Walkerburn, UK). The water used was deionized of MilliQ grade.

Sample preparation
Homogenized solid samples (approx. 2 g) of fish fillet, shrimp, zooplankton, liver, sediment and sludge (centrifuged) were extracted with hexane and 90% acetonitrile twice by vortex mixing for 3 min and centrifugation at 2500 g for 5 min between extractions. The two hexane extracts were then combined in a volumetric tube and the volume adjusted to 10 ml with hexane. Water samples were extracted with equal volumes of cyclohexane and the organic phase reduced to 1 ml by evaporation with N_2.

Super critical fluid chromatography coupled to tandem mass spectrometry (UPC2-MSMS)
Super critical fluid chromatography was performed on a HSS C18 column (1,8 µm, 100 mm × 3 mm) (Waters, Milford, MA, USA), using a Waters Acquity UPC2 module. Separation was achieved by using a linear gradient elution at 1.2 ml/min starting with 98% A (CO_2) and 2% B (MeOH/ACN, 1/1, containing 1 g/L ammonium formate) rising to 50% B over 7 min. and maintained for 5 min before the eluent was switched back to 2% B. The UPC2 system was coupled to a Quattro Premiere triple quadrupole mass spectrometer (MS) operating with an ESI interface (Waters Micromass, Manchester, UK). ESI parameters were a spray voltage of 3.5 kV, desolvation temperature at 400 °C, source temperature at 120 °C and cone gas and desolvation gas at 50 and 800 L/hr of N_2, respectively. Make up flow was 0.25 ml/min MeOH with 0.2% formic acid. The mass spectrometer was operated in MS/MS mode with argon as the collision cell gas at 1.3×10^{-3} Torr. Ionization and MS/MS collision energy settings were optimized while continuously infusing (syringe pump) 100 ng/ml of individual phosphite standards at a flow rate of 10 µl/min. Screening of phosphite were performed with multiple reaction monitoring (MRM) in positive ionization mode using the $(M+H)^+$ adducts and 2 mass transitions were used for each phosphite compound. The organic phosphites were quantified using external calibration curve of standard specimens disolved in hexane.

Method Validation
Control fish fillet of trout (2 g) and shrimp (2 g) were fortified to give concentrations of 20, 50 and 100 ng of each phosphite/g sample. These samples were analysed in triplicate using the method described above.

Standard addition samples were run with each series of samples. Recoveries were generally good at between 60 and 100% in most matrices and for most compounds. However in certain matrices, especially the liver samples, there was low recovery for several of the phosphites. The phosphites were rapidly transformed, possibly to their oxidized products, the corresponding phosphates. Phosphate standards were not run with the samples, but MRM traces corresponded to the phosphate esters of triisodecyl phosphite, triphenyl phosphite, Irgafos 126 and triisotridecyl phosphite were included in the method and peaks corresponding to these were abundant in the phosphite spiked samples suggesting that this is the case.

Determination of LOQ
LOD were calculated using signal/noise ratio of 3 and LOQ with signal/noise ratio 10. Irgafos 168 co-eluted with triglycerides and hence has a higher LOQ in fatty tissues such as liver and fatty fish. The high LOQ for tris(2,4-ditert-butylphenyl) phosphite in the water samples was due to trace levels of this phosphite in the organic solvent used for extraction (cyclohexane) and the 500 X concentration of the cyclohexane extract.

Table 5: Recoveries (%) of selected organic phosphites from trout fillet, shrimp and solvent.

	Spiked material								
	Trout fillet			Shrimp			Solvent		
Compound	20 ng/g	50 ng/g	100 ng/g	20 ng/g	50 ng/g	100 ng/g	20 ng/L	50 ng/L	100 ng/L
Irgafos 168	nd	75	81	110	125	135	75	86	85
tris(2,4-ditert-butylphenyl) phosphite	102	104	97	131	118	89	105	109	105
triisodecyl phosphite	78	105	105	91	127	126	73	70	72
tris(nonylphenyl) phosphite	83	96	100	82	115	100	89	98	99
triphenyl phosphite	107	104	102	105	109	104	90	100	91
Irgafos 126	86	111	100	76	87	87	108	108	113
isodecyl diphenyl phosphite	101	109	96	94	106	100	87	106	100
triisotridecyl phosphite	76	112	104	87	125	120	74	71	78
2-ethylhexyl diphenyl phosphite	91	99	113	90	102	102	88	90	88
diisodecyl phenyl phosphite	86	106	102	95	115	107	70	88	91

2.2.2 PBT compounds

Materials and General Remarks
Standards (BHT, PBO, DBT, AO2246, Octabenzone, TTBNPP, and MDI) and internal standards (d_{15} TEP, d_{27} TBP and d_{15} TPP) were purchased from Sigma. Solvents, adsorbents and SPE were purchased from VWR, Oslo, Norway.

Special precautions for sample preparation and the cleanup of samples are important to decrease background levels of PFRs. All glassware was heated to 450 °C before use and washed with acetone. Metallic spoons were sonicated in acetone, while solid phase cartridges were thoroughly washed with the strongest eluent.

Sample Preparation and Extraction
Biological samples
Two grams of sample was homogenized in anhydrous Na_2SO_4, and placed in an extraction column, and internal standard added and extracted using a solvent of ethylacetate/cyclohexane. The extract was concentrated and liquid-liquid partition extraction performed using n-hexane and acetonitrile. The n-hexane phase was discarded while the acetonitrile fraction was further cleaned using SPE using Supelclean™ PSA and the analytes extracted using methyl tert-butyl ether. The sample was concentrated to dryness and 0.5 ml of toluene added and transferred to analytical vials.

Sediment and particle samples
Sediment samples were dried before extraction at 35 °C until constant weight. Internal standard was added and the sample soxhlet extracted using ethylacetate/cyclohexane for 8 hr with activated copper in the collection vessel. Samples were concentrated and cleaned-up using activated florisil and the analytes collected using etylacetate/cyclohexane. The extract was concentrated and transferred to vials for analysis. Particles from water samples were filtered out on a microfiber filter GF/C. The filter was dried at 35 °C and extraction and clean-up was done as for the sediment samples.

Water samples
Water samples (150-250 ml), containing the internal standard, were extracted by SPE using pre-conditioned Strata-X columns. Following extraction the cartridges were dried and the analytes eluted using dichloromethane. The samples were concentrated and transferred to vials for analysis.

Analysis
Analysis of BHT, PBO, DBT, AO2246, and octabenzone were performed on an Agilent 5973MSD GC/MS system using a Restek Sil5-MS GC-column. TTBNPP and MDI were analyzed on an Agilent 6550 LC/MS-QToF system.

2.2.3 Non-target screening

Extraction and clean-up methods
Following reception and registration, the samples were stored frozen at -20 °C until extraction and clean up. To cover the broadest possible range of compound groups two different extraction and clean-up methods were applied. One method was optimized for non-polar and very lipophilic compounds such as PCBs, PAHs and other classical POPs. Another method was optimized for polar compounds such as pharmaceuticals, modern pesticides and biocides, PFCs, and bisphenols.

Prior to extraction samples were spiked with a number of isotopically labelled internal standards, that in the future will enable the retrospective semi-quantitative determination of selected compounds.

Extraction of polar compounds

The extraction of polar compounds used the same method as for organic phosphite analysis described above. Homogenized samples (approx. 2 g) were extracted with hexane and 90% acetonitrile twice by vortex mixing for 3 min and centrifugation at 2500 g for 5 min between extractions. The two acetonitrile extracts were then combined, and extracts were analysed by liquid chromatography. The hexane extracts were analysed for organic phosphites.

Extraction of less polar compounds

Two grams of sample was homogenized in anhydrous Na_2SO_4, placed in an extraction column, and internal standard added and extracted using a solvent of ethylacetate/cyclohexane. The extract was concentrated and cleaned-up using (1) activated florisil and (2) C18/Z-sep(+). For lipid rich samples GPC on BioBeads SX-3 was applied before the florisil/C18/Z-sep clean-up.

Selection of instrumental analytical methods

Figure 4 shows schematically the application range of the different available MS-techniques, and it is obvious that only the combined application of both GC- and LC-MS will provide sufficient coverage for the majority of possible environmental pollutants.

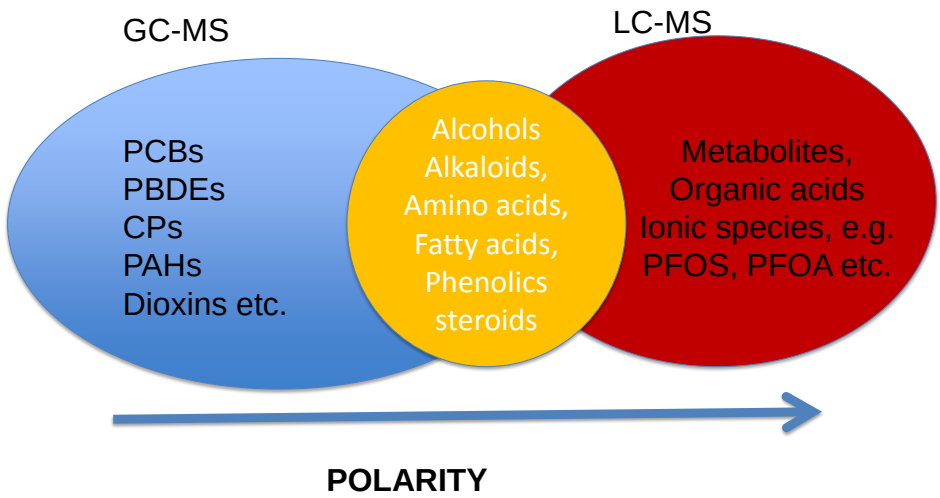


Figure 4: Application range for GC-MS and LC-MS techniques

To cover the broadest possible range of non- and semi-polar compounds GCxGC/LRToF in electron ionization (EI) (NILU) and GC/HRToF in electron ionization (EI) (NIVA) were used. For the semi-polar and polar range of compounds samples were analysed with LC/HR-qToF technique in both positive and negative ESI-mode. NIVA was responsible for negative ESI, and NILU for positive ESI. The most important advantages of the application of high resolution ToF techniques are ultimate sensitivity and exact mass detection, which allow the determination of the molecular formula, which is important for substances not registered in mass spectral libraries.

Full scan analysis with GCxGC-LRToF in EI

All matrices (excluding the rats) were analysed by a Leco GCxGC-LRToF MS operated in EI mode at low resolution. The GCxGC/ToF-MS system consisted of a Pegasus® 4D (LECO, St.

Joseph, MI) system equipped with a Restek (Bellefonte,PA, USA) Rxi-5Sil-MS (30 m, 0.25 mm x 0.25 µm) as the first dimension column and a SGE (SGE Internat. Pty Ltd., Australia) BPX-50 (1 m, 0.1 mm x 0.1 µm) as the second dimension column. Helium (purity 99.9990%, Hydro Gas and Chemicals, Oslo, Norway) was used as carrier gas with a constant flow of 1.4 mL/min. 1 µL of each extract were injected in Pulsed Splitless Mode with a pulse pressure of 50 psi for 1.5 min with an Agilent split-/ splitless injector. The injector temperature was set to 280 °C with a purge time of 180 s and purge flow of 50 mL/min.

The primary GC column was programmed as follows: 80 °C (hold time 2 min) and ramped at 10 °C/min to 300 °C (hold time 10 min). The secondary oven temperature was programmed 100 °C (hold time 4 min) and ramped at 10 °C/min to 315 °C (hold time 8.5 min). The modulation period was set to 2.2 s with 0.66 s hot pulse time and 65 °C modulator temperature offset relative to the primary oven temperature. Liquid N_2 was used as the coolant of the GCxGC modulator. The ion source and the transfer line temperatures were set to 200 °C and 250 °C, respectively. The electron energy was 70 eV and the detector voltage was 1850 V. A data acquisition rate of 250 spectra/s was used in combination with an acquired mass range of 33 – 1000 u. Autotuning was performed by using the m/z 219 perfluorotibutylamine (PFTBA) ion instead of the default m/z 69 ion. In order to avoid system contamination, the glass liner was changed after each injection followed by solvent clean runs (5x toluene and 2x isooctane).

Full scan analysis with GC-HRToF in EI
An aliquot of the sample extract was analysed by GC-HRToF MS operated in EI mode with high mass resolution (>8500).

Extracts (1 µl) were injected into an Agilent gas chromatograph fitted with a 30 m × 0.25 mm, 0.25 µm film thickness DB-5MS column (Agilent Technologies) with helium carrier gas at a constant flow of 1 ml/min and a splitless injection at 250 °C. The initial over temperature of 60 °C was held for 2 min, followed by an increase of 6 °C/min to 310 °C and held for 10 minutes. The GC was coupled to high-resolution time-of-flight mass spectrometer (GCT Premier, Waters Corp, Milford MA, USA) that was operated in full scan positive electron impact mode with a scan range of 50−500 m/z from 9 to 50 minutes run time. The source temperature was 200 °C and the electron energy, 70 eV, and the resolution was 8500.

Data Processing
Screening and non-target data processing performed with ChromaLynx software from Waters (Milford, USA) and the NIST library (http://www.nist.gov/nvl/) based 4 ions of interest. Peak confirmation used the elemental composition function using an acceptance criterion of 5 mDa error on a minimum of 3 dominant ions.

Full scan analysis with LC-HR-QToF in positive ESI-mode
An aliquot of the sample extract was analysed using an Agilent 1290 UHPLC system with an Accucore Polar (250mm x 2.1 mm, 2.6 µm) column (Thermo Scientific) coupled with Agilent 6550 HR-QTOF- with Dual Jet Stream electrospray source operating in the positive mode. A 32 min gradient of mobile phases: A (water with 0.1% formic acid) and B (methanol) was used to enable the separation of a broad range of compounds with different physic-chemical properties. The detector operated in the range of 25-1700 Da, with gas temperature 200 °C, drying gas 18 l/min, nebulizer 30 psi, sheath gas temperature 300 °C and sheath gas flow 12 l/min. To ensure maximum sensitivity of the method for compounds being on the list of

targets and suspects all samples were analysed first in a full scan MS mode. Afterwards sample were reanalysed in a MSMS mode with different collision energies to facilitate sufficient confirmation of the compounds from the suspect list and tentative identification of unknown compounds.

The data was processed with various modules being the part of Agilent Mass Hunter data processing platform (ver. B.07).

Analysis with LC-HR-QToF in negative ESI-mode
An aliquot of the sample extract was subjected to instrumental analysis with a UHPLC-HR-QTOF-MS with electrospray ionization operating in negative mode. This will enable detection of the substances that are sufficiently acidic to lose a proton and contain for example carboxyl groups (e.g. PFAs) or phenolic groups (e.g. bisphenols).

Chromatography
Acquity UPLC system with an Acquity BEH C18 (2.1 x 100 mm) column (both from Waters Corp, Milford USA). A gradient mobile-phase was run from 2% methanol (with 10 mM ammonium acetate) to 98% methanol (with 10 mM ammonium acetate) over 12 minutes with a flow of 0.45 mL/min. The mobile phase was held at 98% methanol (with 10 mM ammonium acetate) for 1 minute to wash the column before returning to starting conditions for reequilibration. Total run-time was 15 minutes and the sample injection volume was 5 µL.

Mass Spectrometry
The detector was a Xevo G2-S QTOF (Waters Corp. Milford USA) operating in electrospray-negative mode over the range 50 - 1000 Da. Data-acquisition was with 3 channels; (1) Low energy channel for molecular ion detection, (2) High energy channel for detection and identification of fragment ions (pseudo-MSMS), (3) Lock-mass channel for online continuous mass-calibration. Capillary Voltage 0.7 kV, Cone Voltage 25 V, Desolvation temperature 450 ^{o}C, Desolvation gas flow (N_2) 1000 L/hour and source temperature 100 ^{o}C.

Data Processing
Screening and non-target data processing was performed using the Unifi software (v1.7) from Waters (Milford, USA). Taking into account that extract contains a very broad range of semi-polar and polar compounds, chromatographic method were optimised to ensure maximum separation in the whole range of polarity. To ensure maximum sensitivity of the method for compounds being on the list of targets and suspects all samples were analysed first in a full scan MS mode. Afterwards sample were reanalysed in a MSMS mode with at least 3 different collision energies to facilitate sufficient confirmation of the compounds from the suspect list and tentative identification of unknown compounds.

2.2.4 Data treatment

Full scan analyses conducted on high resolution mass spectrometers allow to obtain and register enormous amount of information so MS-peak picking algorithms will normally find thousands of compounds in a sample, containing chemical background, normal matrix components and different compounds of interest. The majority of these peaks will be “natural” chemical compounds and the challenge is to identify relevant environmental pollutants. It would be impossible to investigate every single peak effectively and efficiently, and many of those peaks may be of little interest. For example, natural substances like

sugars, amino acids and nutrients are of minor interest when looking for environmental pollutants.

During the last five years, 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 have been developed. The NORMAN network (http://www.norman-network.net/) is a driving force in this development with the project group as an important contributor to this collaboration. As the latest and most import step in this development an interlaboratory study (ILS) was organized which was finalized with an international workshop. NILU and NIVA, together with 15 other European laboratories have participated and the outcome of the ILS and workshop discussions are accepted in a peer-review journal (Schymanski et al., 2015). One of the major outcomes of this meeting was a general consensus to use a workflow protocol proposed by Eawag (Schymanski et al., 2014) for acquisition and data treatment of non-target high resolution mass spec data. A detailed explanation of the workflow and further other details are given in the cited reference. With low-resolution data it is not possible to estimate molecular formulas and therefore the workflow was slightly different as shown in Figure 5.

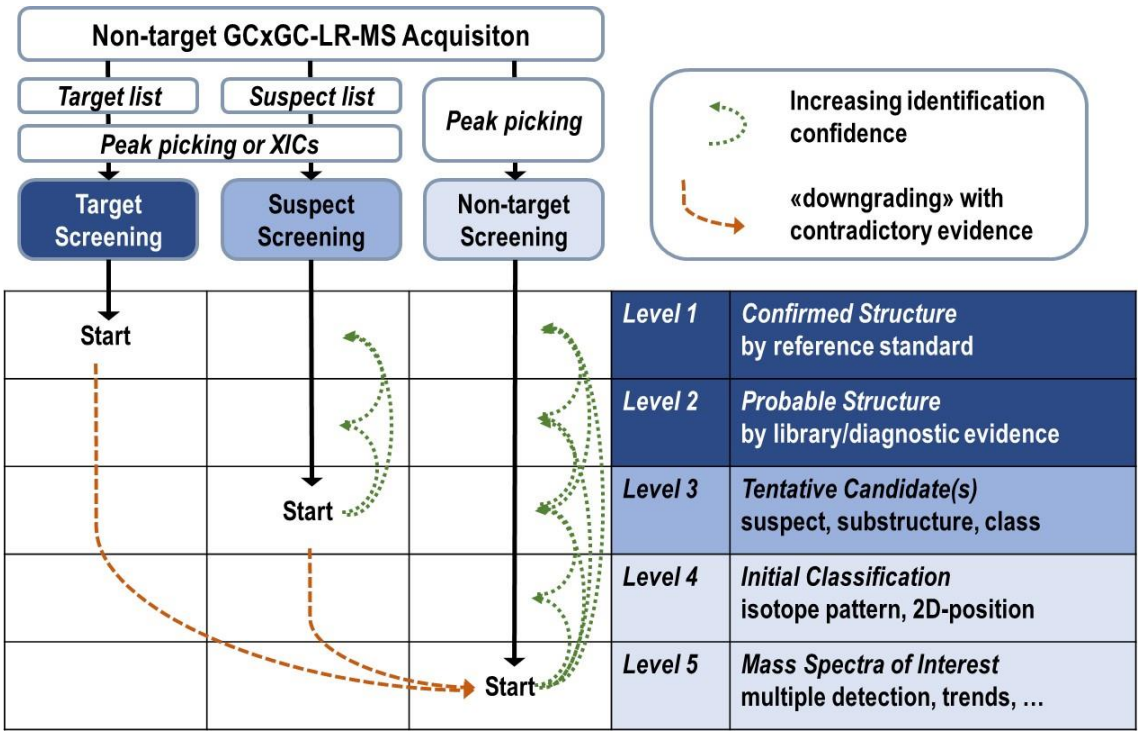


Figure 5: Workflow and identification confidence for methods with low mass resolution. Adapted from (Schymanski et al., 2014).

2.3 Supporting parameters

2.3.1 Particle Size Analysis

Wet sediment was shaken by mechanical fractionater fitted with < 63 µm sieves. Dry weight measurements were used for the particle size calculations.

2.3.2 Sediment TOC

Freeze dried sediment sample aliquots (0.5-10 mg) were heated in a furnace at 1,800 °C in the presence of oxygen free helium. The carbon dioxide gas produced was passed through a chromatography column and the total organic carbon was measured.

2.3.3 Water DOC

Samples (4 ml) were injected into an inorganic carbon chamber and 0.5 ml 21% phosphoric acid was added. The inorganic bound carbon from carbonates, bicarbonates and dissolved CO_2 is released to an NDIR detector for CO_2 quantification.

2.3.4 Lipid content

An aliquot of homogenised biota (approx 2 g) was weighed. 40 ml of cyclohexane/isopropanol (50/50) was added and the samples shaken for 2 hours. The samples were centrifuged at 2000 g for 10 minutes. The solvent phase was decanted into a clean tube and the extraction repeated with 30 ml of cyclohexane/isopropanol (50/50) and the extracts combined. 20 ml of 0.5% NaCl was added to the combined extracts and shaken before again centrifuging at 2000 g for 10 minutes. The cyclohexane layer was transferred to pre-weighed tubes and then evaporated under nitrogen. When the cyclohexane had been removed the tubes were heated at 60 °C to a constant weight (approx 24 hrs) and the lipid content calculated.

2.3.5 $\delta^{13}C/\delta^{13}N$ ratio analysis

Samples were dried at 60 °C for 24 hours before grinding to fine powder. Approx 1 mg of sample was combusted in the presence of O_2 and Cr_2O_3 at 1700 °C in a Eurovector element analyser. Reduction of NO_x to N_2 was done in a Cu oven at 650 °C. H_2O was removed in a chemical trap of $Mg(ClO_4)_2$ before separation of N_2 and CO_2 on a 2 m Porapolt Q GC column. The C/N ratio was quantified on the basis of the m/z 44/28 ratio. N_2 and CO_2 were directly injected online to an isotope ratio mass spectrometer (Nu Instruments Horizon) for the determination of $\delta^{13}C$ and $\delta^{13}N$. The mean stable N-isotope ratios, δ15N, reflect the relative trophic position of the organisms. Likewise, the stable C-isotope ratio, δ13C, reflects the carbon sources of the organism. A low $\delta^{13}C/\delta^{13}N$ ratio indicates influence from a pelagic food chain whereas a higher ratio indicates a more littoral food chain. We have lipid-adjusted all the δ13C-ratios in order to remove the effect of 13C-depleted lipids in the fatty burbot samples.

2.4 Uncertainties

When performing environmental screening studies for contaminants of emerging concern, all steps in the process, starting with study design, selection of the sampling sites, sampling frequency, time of sampling, performing the sampling, the transport and storage of samples, chemical analysis and data treatment, to some extent generate some degree of uncertainty. To estimate quantitatively the contribution of all steps is an extreme difficult task. However, we estimate that the uncertainty for such screening analysis are higher than for routine monitoring of PCBs or other “classical” POPS. Whereas we expect a total expanded measurement uncertainty of about 25 to 30 % for PCBs, this value might be as high as 40 to 50 % for new emerging compounds as measured in these report.

3. Results and Discussion

None of the selected organic phosphites were detected at concentrations above the limits of detection in any of the samples analysed. The absence of organic phosphites in the environment may possibly be due to a low level of release from products or that they rapidly transform (or a combination of the two factors). This section will therefore focus on the results from the analysis of selected PBT substances.

3.1 Wastewater treatment works effluent

From the selected PBT substances only BHT and PBO were detected in effluent at a range of between <LOD and 1,200 ng/L (Figure 6). BHT was detected in all effluent samples at between 166 and 1,200 ng/L. The highest concentrations were detected in the samples from Tomasjord (525 – 1,200 ng/L), and slightly lower in samples from VEAS (166 – 857 ng/L) and HIAS (374 – 451 ng/L). In comparison, somewhat lower BHT-concentrations were found in a German survey from 2004, with BHT concentrations in sewage influent at between 263 and 478 ng/L and sewage effluent at between 22 and 258 ng/L (Fries and Püttmann, 2004). In a recent study of sewage effluent from Beijing, China, slightly higher BHT concentrations were measured (2,120 - 2,510 ng/L; Liu et al., 2015). River water upstream to this source showed a concentration of around 100 ng/L, but downstream between 500 and 1,115 ng/L.

PBO was detected in all but one effluent samples in the range of LoD to 782 ng/L. The highest concentration was found in one sample for HIAS. PBO was earlier found in STP effluent in Spain in the range of below LoD to 40 ng/L (Rodil et al., 2012).

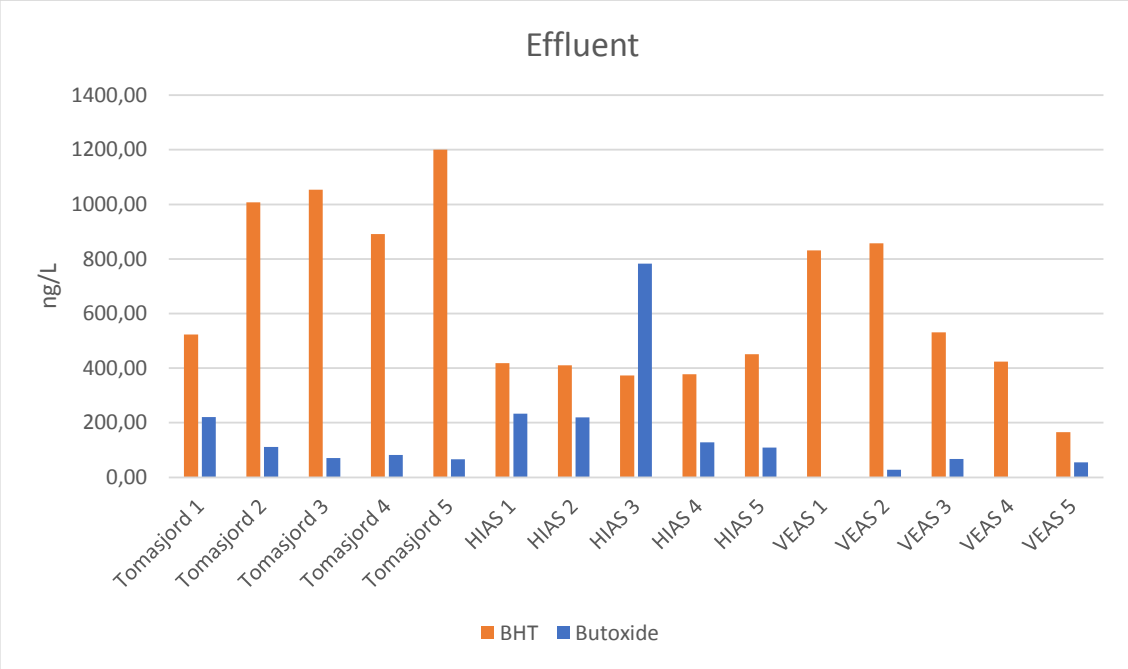


Figure 6: Concentrations of selected PBT compounds in WWTW effluent

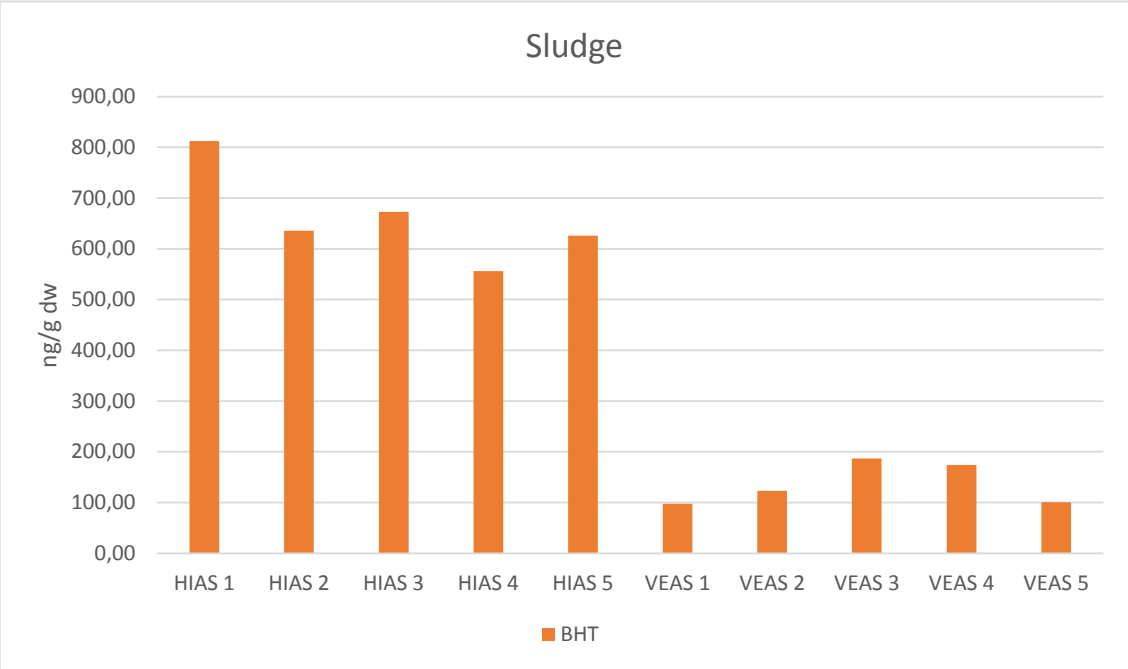


Figure 7: Concentrations of selected PBT compounds in sludge

In sludge samples only BHT was detected above the LoD (Figure 7). The concentrations ranged from 98 – 187 ng/g dw in samples from VEAS and from 556 – 812 ng/g dw in samples from HIAS. In a recent study at a Beijing STP higher concentrations were found 1,400 – 2,325 ng/g dw (Liu et al., 2015). However, these samples were undigested sludge from the dewatering step very early in the sludge treatment process. BHT has shown to be biodegradable in sludge treatment (Boonnorat et al., 2014) which may explain these differences.

3.2 Leachate

3.2.1 Selected PBT substances

From the individual PBT substances in leachate only BHT was measured at concentrations above LoD in a range of between 200 – 1,390 ng/L in the filtrated water phase (Figure 8) and 82 – 730 ng/L in the corresponding particle phase (Figure 9).

The concentrations of BHT in the leachate both in the water and in the particle phase are slightly higher in samples from Lindum compared to ISI. If this can be attributed to the fact that ISI was closed down already in 2003 and Lindum is still in use as a solid waste landfill or if this is only reflecting natural variations in drainage and water flow is difficult to decide with such few measurements. However, the concentrations measured in this study are several orders of magnitude lower than what was measured at solid waste dump site in Thailand where concentrations of 100 µg/L have been reported (Boonnorat et al., 2014).

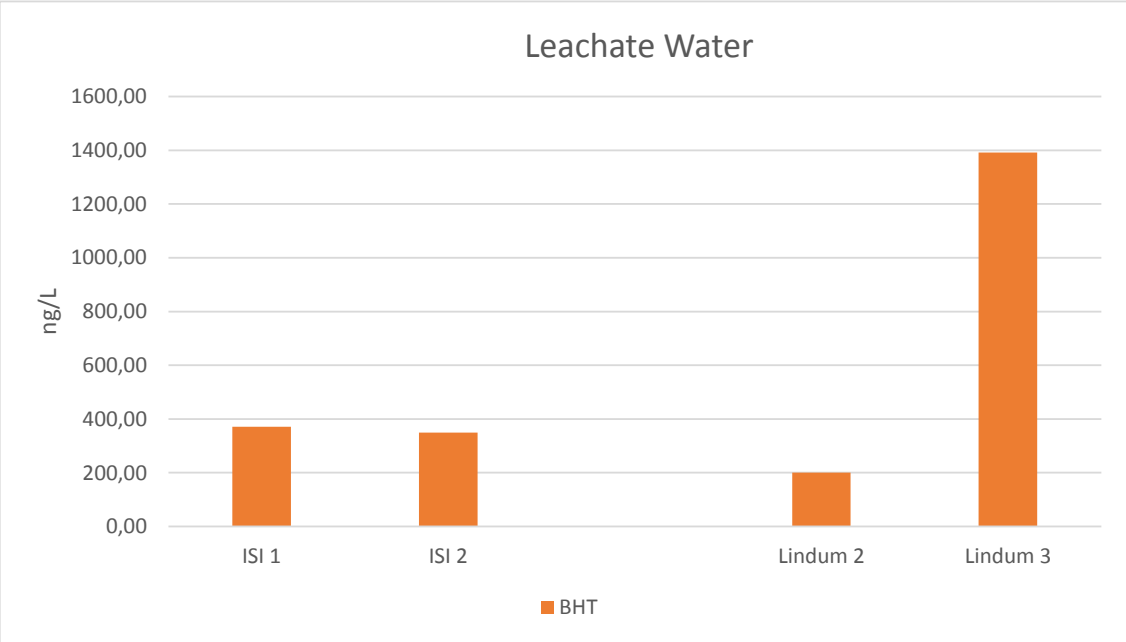


Figure 8: Concentrations (ng/L) of BHT in leachate liquid phase (Analysis of Lindum 1 failed and was not possible to repeat).

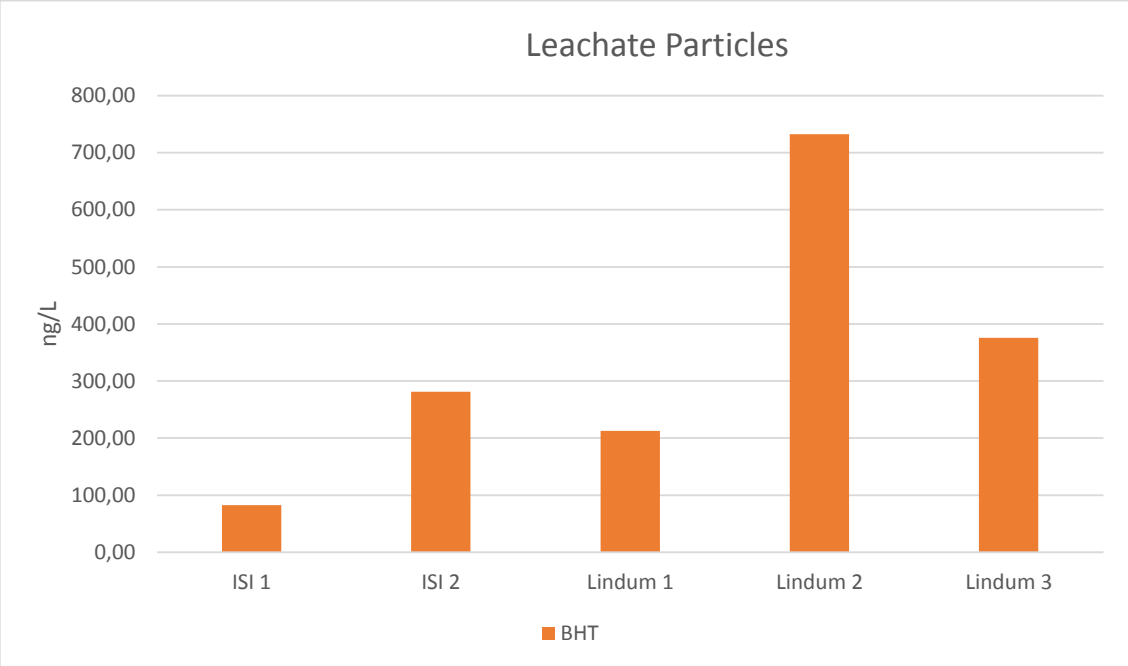


Figure 9: Concentrations (ng/L) of BHT in leachate particles.

3.3 Oslofjord and Lake Mjøsa Sediment

3.3.1 Selected PBT substances

From the individual PBT substances only BHT was measured at concentrations above LoD in a range of between 22 – 102 ng/g dw in sediments from Oslofjord and 18 – 94 ng/g dw in

sediments from Lake Mjøsa (Figure 10). These concentrations are comparable to measurements from an industrialized area in Greece (LoD – 840; Grigoriadou and Schwarzbauer, 2011).

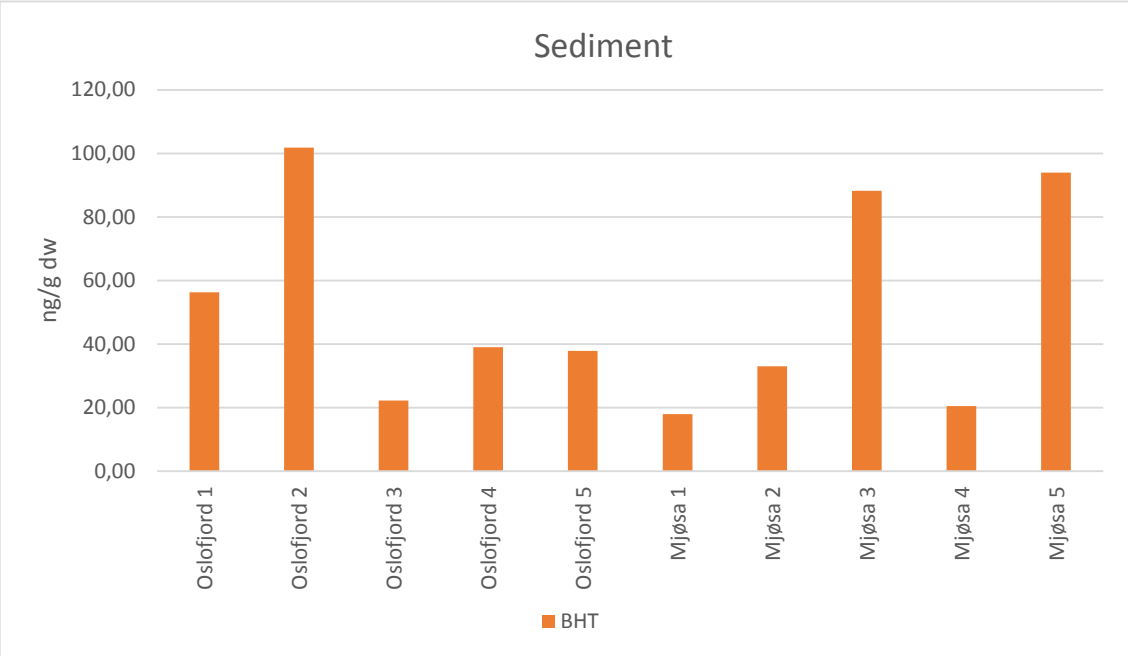


Figure 10: Concentration of BHT in Oslofjord and Lake Mjøsa sediments.

3.4 Oslofjord biota

3.4.1 Selected PBT substances

Of the selected PBT substances, only BHT (and the reference analyte PCB-153) was detected in biota samples from Oslofjord. The BHT concentrations were in the range of 0.6 – 9.9 ng/g fw for Krill, 0.4 – 2.4 ng/g fw for Northern shrimps, 0.5 – 4.3 ng/g fw for Herring, and 0.5 – 12 ng/g fw for Cod liver (Figures 11 to 14). The PCB-153 concentrations were in the range of 2.4 – 3.9 ng/g fw for Krill, 2.1 – 3.1 ng/g fw for Northern shrimps, 13 – 87 ng/g fw for Herring, and 600 – 1,940 ng/g fw for Cod liver (Figure 11 - Figure 14).

In a recent study of farmed fish, high levels of BHT and other antioxidants were found, with BHT levels of up to 7.6 µg/g fw in farmed Atlantic salmon fillet (Lundebye et al., 2010). These levels can be attributed to the extended use of antioxidants in fish feed which give a high and direct exposure of the farmed fish to these compounds. The authors calculated that one 300 g portion of farmed Atlantic salmon would contribute up to 75% of the acceptable daily intake (ADI) for BHT.

With the exception of herring, the sample-to-sample variation within each sample matrix is much lower for PCB-153 than for BHT. This might be due to a much faster excretion or metabolism of BHT compared to PCB-153. In this case high concentrations of BHT in a sample might reflect recent uptake only, whereas the level of the very persistent PCB-153 is more dominated by the uptake over the whole live time of the individual animal.

The different selected sample types are coming from both low and high trophic levels. However, the concentration range of BHT in all sample types are nearly identical, and thus, the selected marine food chain is not giving evidence for biomagnification of BHT throughout the food chain.

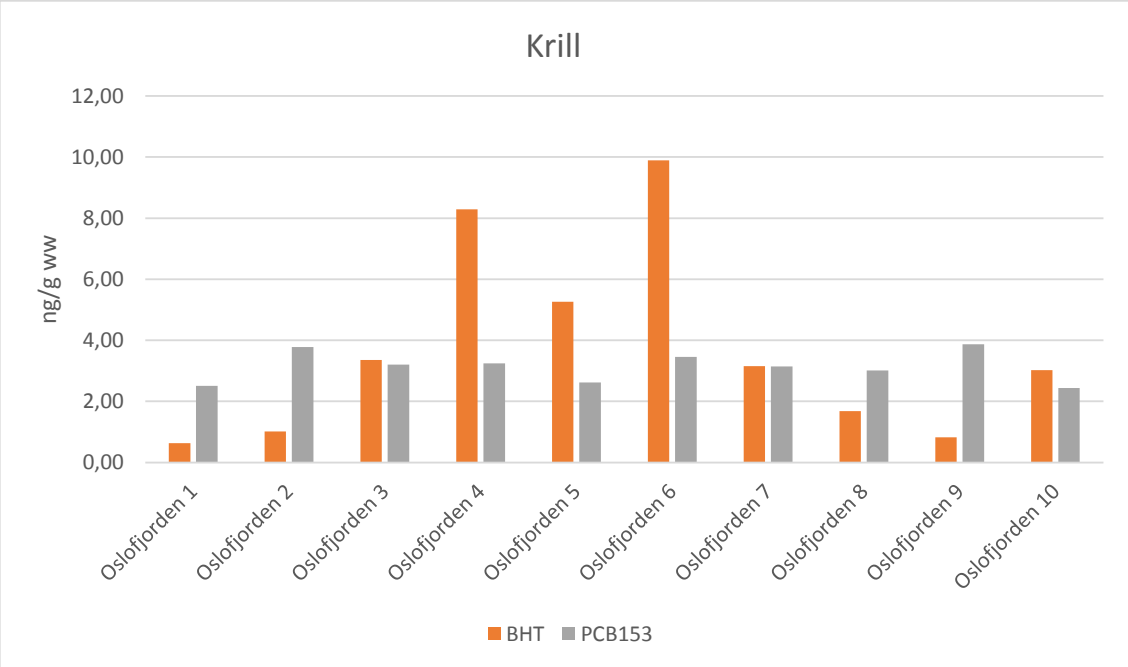


Figure 11: Concentrations of BHT in Krill from Oslofjord.

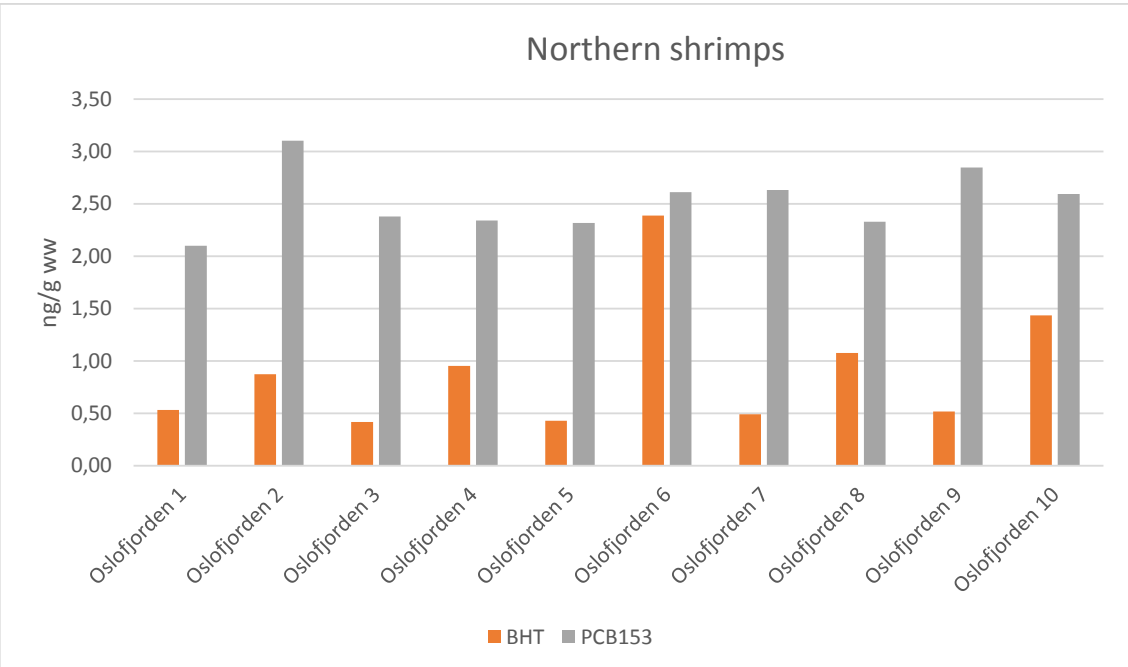


Figure 12: Concentrations of BHT in Northern shrimp from Oslofjord.

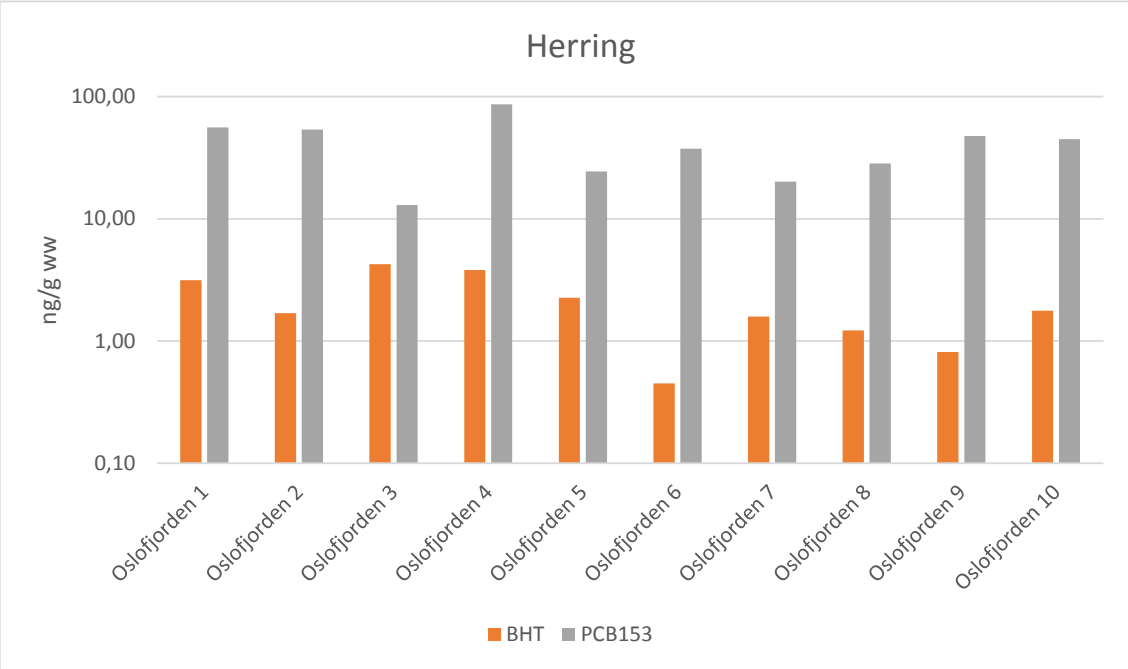


Figure 13: Logarithmic concentrations of BHT & PCB153 in herring from Oslofjord.

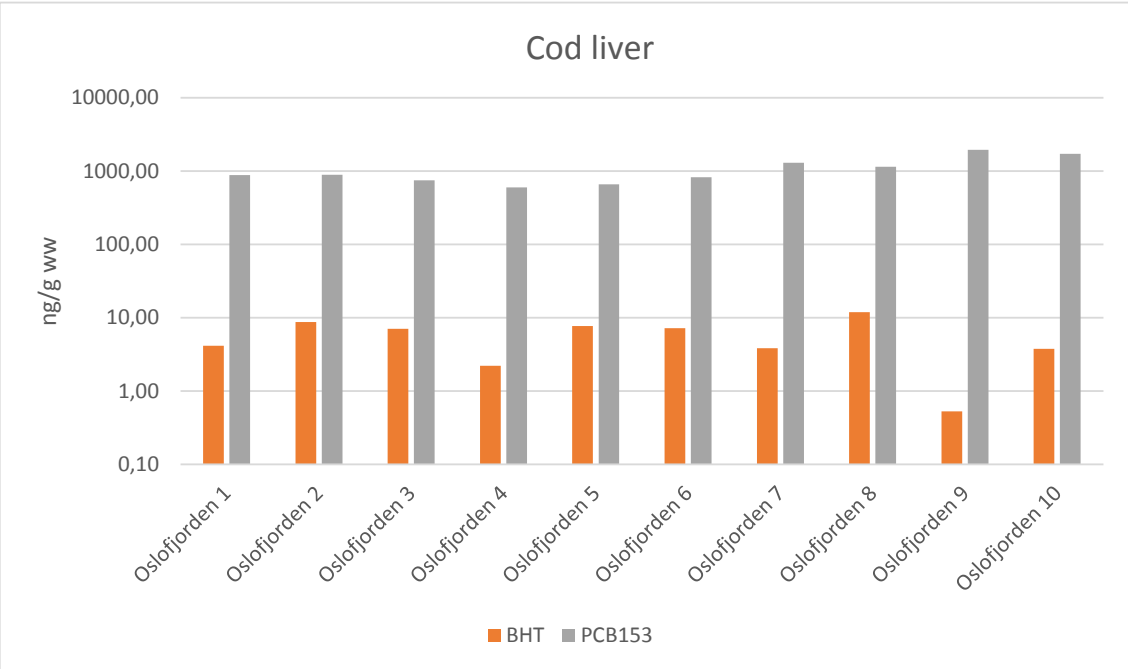


Figure 14: Logarithmic concentrations of BHT and PCB153 in cod liver from Oslofjord.

3.4.2 Biomagnification of BHT and PCB153

Inspection of pairwise scatterplots between BHT and PCB153 concentrations (lipid weight) and isotopic ratios ($\delta^{15}N$ and $\delta^{13}C$) revealed that BHT did not accumulate in the food chain, but rather showed sign of biodilution at higher trophic levels (Figure 15). This is contrary to PCB153 for which the concentrations were elevated in cod liver compared to crustaceans and

herring. The scatterplot between N- and C-isotope ratios showed that krill and herring relied on a more ^{13}C-depleted food source than shrimp and cod. This may be indicative of a more pelagic habitat for krill and herring as compared to shrimp and cod, which are more associated to a benthic/littoral habitat. Also, the N-isotope signatures indicated that shrimp and herring occupied approximately the same trophic level —below cod, but above krill.

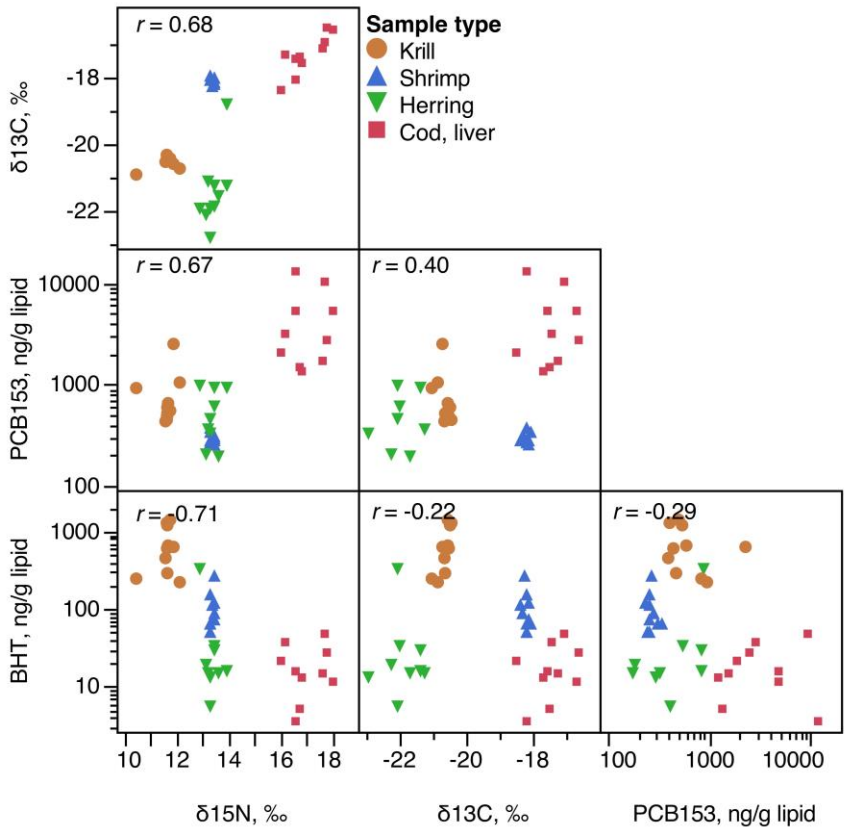


Figure 15: Scatterplot matrix of BHT and PCB153 concentrations (lipid weight) and N- and C-isotope ratios (δ15N and δ13C) in biota samples from Oslofjord. For cod, concentrations refer to liver samples, whereas isotopic ratios refer to muscle samples. The pairwis

Linear regressions of BHT and PCB153 concentrations on N-isotope ratios confirmed that BHT biodiluted in the Oslofjord food web, whereas PCB153 biomagnified as expected (Figure 16). The trophic magnification factor (Borgå et al., 2011) can be defined as the exponential expression TMF = $e^{(b \cdot 3.4)}$. Here b is the regression coefficient for the linear relationship between log-transformed concentrations and $\delta^{15}N$-values of the samples. The multiplication factor of 3.4 reflects the increase in $\delta^{15}N$ from prey to consumer (the enrichment factor per trophic level). A TMF > 1 indicates biomagnification, whereas < 1 indicates biodilution. The TMFs for BHT and PCB153 in the Oslofjord food web were 0.15 and 3.35, respectively, both statistically significant different from 1.

It has been shown that BHT can be produced naturally in freshwater phytoplankton, both green algae and cyanobacteria (Babu and Wu, 2008). It has also been shown that BHT can be produced in marine algae, which may have contributed to the elevated BHT concentrations in pelagic primary consumers, such as krill, but so far we have no further evidence to support this view.

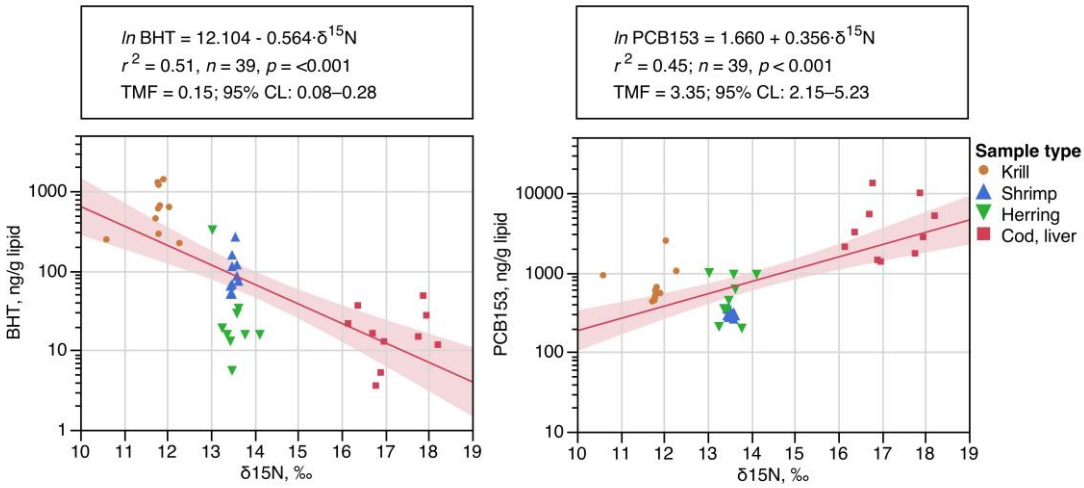


Figure 16: Linear regressions of BHT and PCB153 concentrations (lipid weight) on N-isotope ratios ($\delta^{15}N$) in biota samples from Oslofjord. For cod, concentrations refer to liver samples, whereas N-isotope ratios refer to muscle samples. Regression statistics and trophic magnification factor (TMF) with 95% confidence limits (CL) are given above the plots.

3.4.3 Non-target screening

Confirmed, probabe, and tentatively identified substances (Levels 1 to 3) in the Oslofjord samples are listed in Apendix II. Presentation of the identified substances in the form of a venn diagram (Figure 17, data available in Table 6), shows that 5 compounds are identified in all levels of the Oslofjord foodchain studied; galaxolide (HHCB), hexachlorobiphenyl, p,p´-DDE, PFOS and PFOSA. It is important to note that the certainties behind these identifications differ from compound to compound (Table 6). A further 2 compounds, tonalide (AHTN; a musk xylene) and carbenoxolone (a gastric medicine), were found in all levels of the foodchain apart from cod.

Heaxchlorobiphenyl (PCB congeners 128-169), p,p´-DDE, PFOS and PFOSA are compounds that are know to accululate in biota. The musk xylenes galaxolide and tonalide ar considered an emerging contaminant, however has previously been included in Norwegian Screening projects and is know to bioaccumulate. Little is known about the environmental occurrence of carbenoxolone, however as a level 3 identification, further confirmation is nesseccary.

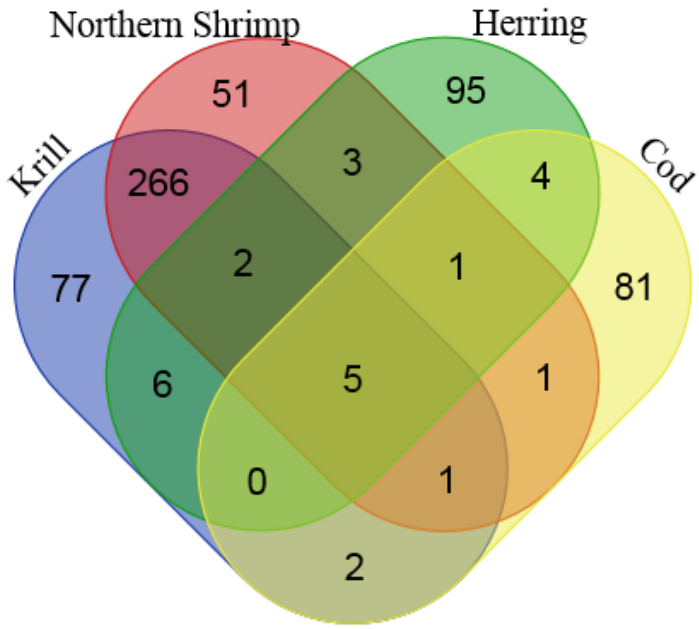


Figure 17: Venn diagram showing all compounds (ID level 1 to 3) found in the different sample matrices from Oslofjord (calculated and drawn with online software by bioinformatics.psb.ugent.be).

Table 6: Summary of non-target screening results by occurrence in the Oslofjord foodchain
ID level in parenthesis

Matrices	No. of compounds	Compounds
Cod, Herring, Krill, Northern Shrimp	5	Galaxolide (1), Hexachlorobiphenyl (PCB 128-169)(1), p,p'-DDE (1), PFOS (3), PFOSA (3)
Herring, Krill, Northern Shrimp	2	Tonalide (3), carbenoxolone (3)
Cod, Krill, Northern Shrimp	1	Diethyl phthalate (2)
Cod, Herring, Northern Shrimp	1	Pentachlorobiphenyl (PCB 82-127)(2)

A heatmap approach to visualise the data clearly shows that the majority of the identifcations are at level 3 (yellow), with very few level 1 identified compounds (red) occurring in all 4 levels of the selected Oslofjord foodchain (Figure 18). The heatmap shows that more successful level 3 and above identifications were made in krill and that these become fewer as one moves up the food chain. This initially would suggest that more chemicals are present in the lower levels of the food chain. However, this should be carefully interpreted, since many of the compounds identified are potentially endogenous and that the greater complexity of the sample matrix in the higher level samples (herring and cod liver) may be interfereing with the analysis and resulting in comparatively fewer positive identifications. What is however clear is that environmental samples from the Oslofjord contain a large number of identifiable compounds.

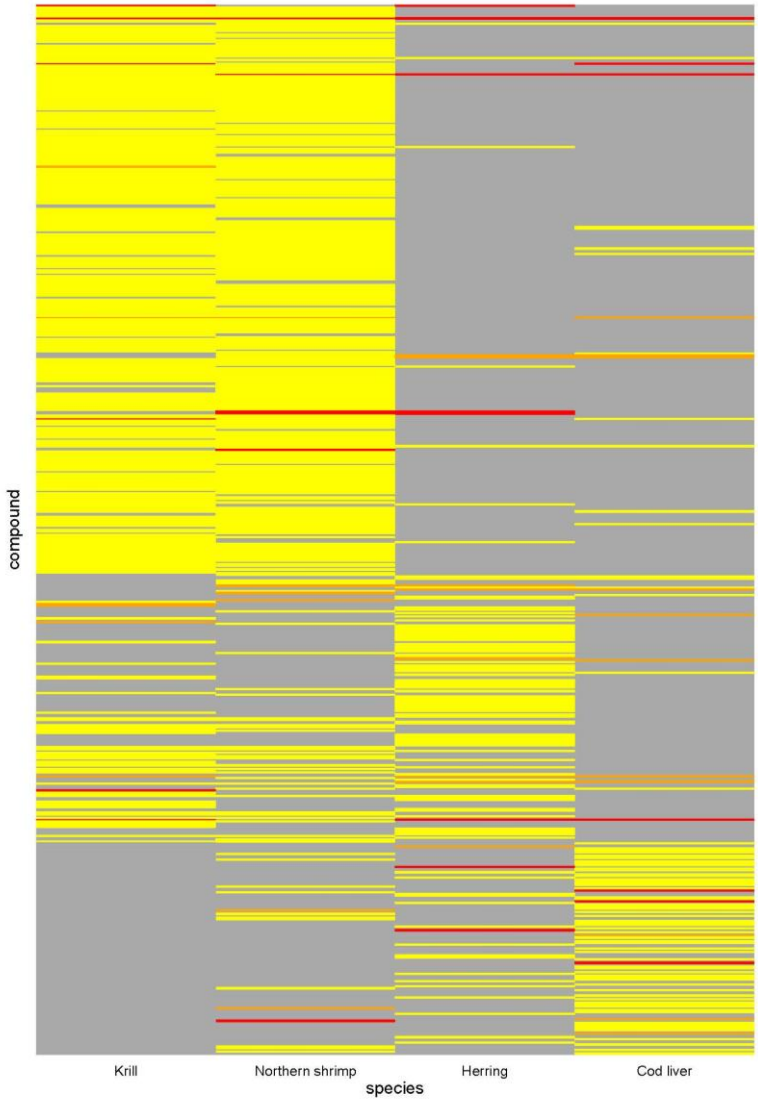


Figure 18: Heat map showing the compounds (Level 3 and above) identified in the Oslofjord samples. Level 1= red, Level 2=orange, Level 3= yellow, Not found= grey).

For the results of this project to be able to inform future screening programmes the first step would be to increase the identification certainty of the high number of level 3 compounds (tenatative candidates) to at least level 2 (probable). As shown in Figure 5, this would involve matching the spectra to available library spectra and/or use further diagnostic evidence. Even better would be the confirmed identity at level 1 through the use of reference standards. This is a major and costly undertaking, but would provide the required further evidence before embarking on a screening programme. All of the level 1 and 2 substances identified in the Oslofjord food chain have already been included in previous screening projects. Carboxolone was identified at level 3 and occuring in the lower three trophic levels of the Oslofjord foodchain. It is therefore recommended to further confirm the identity of this compound as a priority since there is little or no data available on its environmental occurrence.

3.5 Lake Mjøsa biota

3.5.1 Selected PBT compounds

Of the selected PBT substances, only BHT (and the reference compound PCB-153) was detected in biota samples from Lake Mjøsa. The BHT concentrations were in the range of 0.2 – 13 ng/g fw for Mysis, 0.3 – 5.4 ng/g fw for zooplankton, 0.4 – 3.6 ng/g fw for whitefish, 0.6 – 6.6 ng/g fw for smelt, and 0.2 – 1.2 ng/g fw for brown trout (Figure 19 - Figure 23). The PCB-153 concentrations were in the range of 0.4 – 1.9 ng/g fw for Mysis, 0.1 – 1.1 ng/g fw for zooplankton, 1.3 – 4.5 ng/g fw for whitefish, 0.8 – 3.8 ng/g fw for smelt, and 6.9 – 25 ng/g fw for brown trout (Figure 19 - Figure 23).

The different selected sample types are from both low and high trophic levels. However, the concentration range of BHT in all sample types are nearly identical, and thus, the selected freshwater food chain is not giving evidence for biomagnification of BHT throughout the food chain.

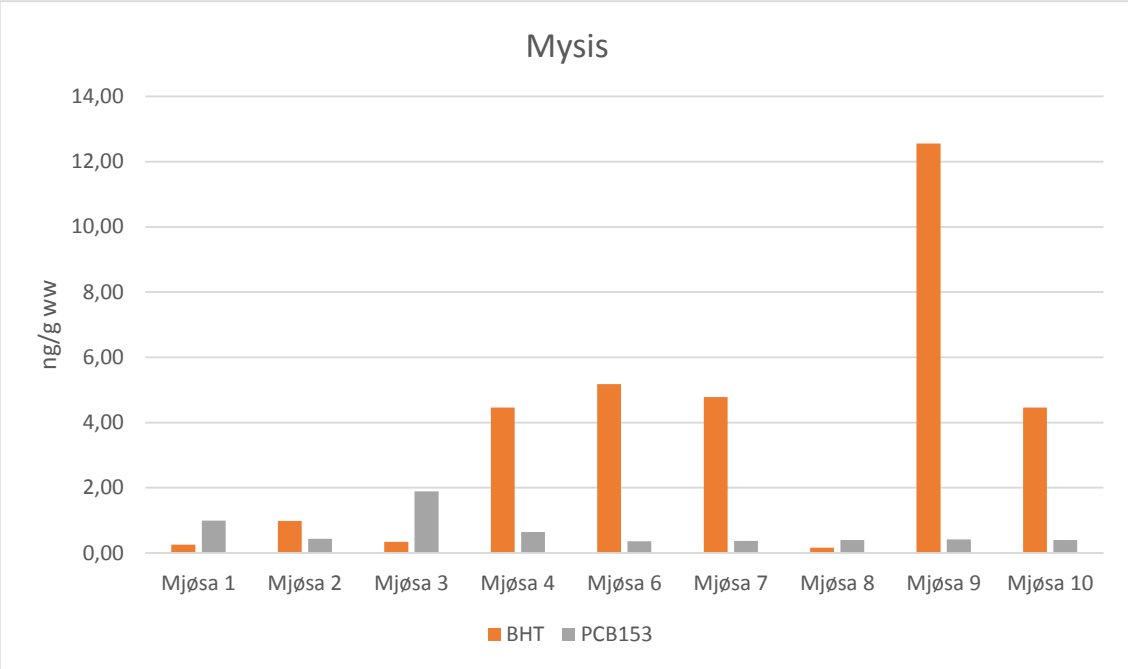


Figure 19: Concentrations of selected PBT compounds in samples of Mysis from Lake Mjøsa.

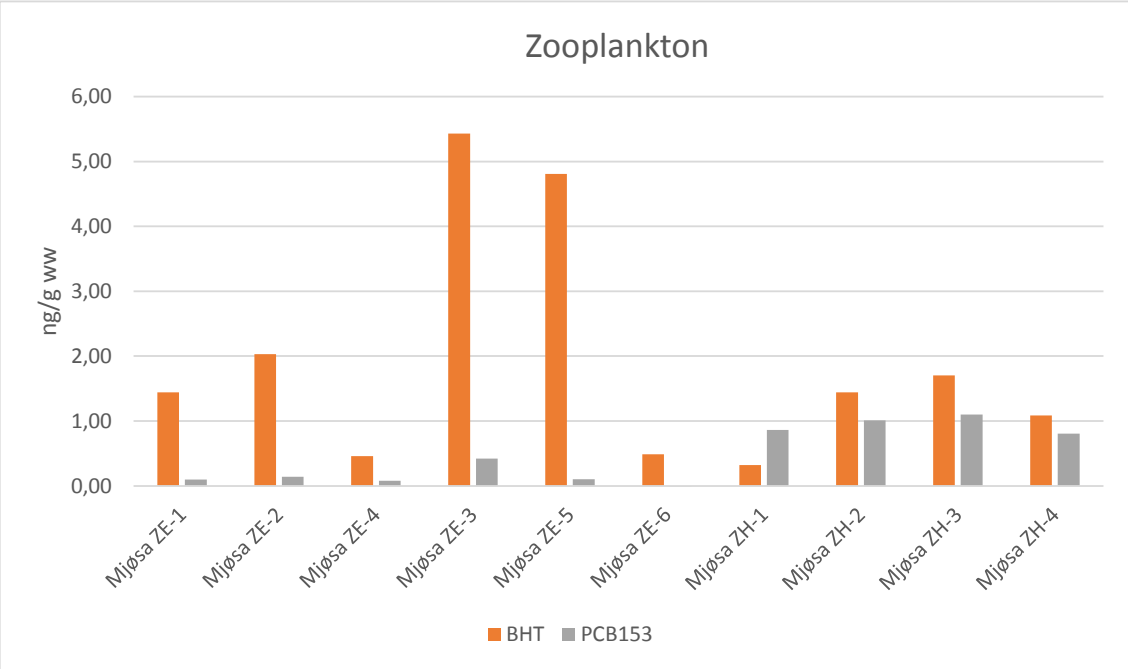


Figure 20: Concentrations of selected PBT compounds in samples of Zooplankton from Lake Mjøsa.

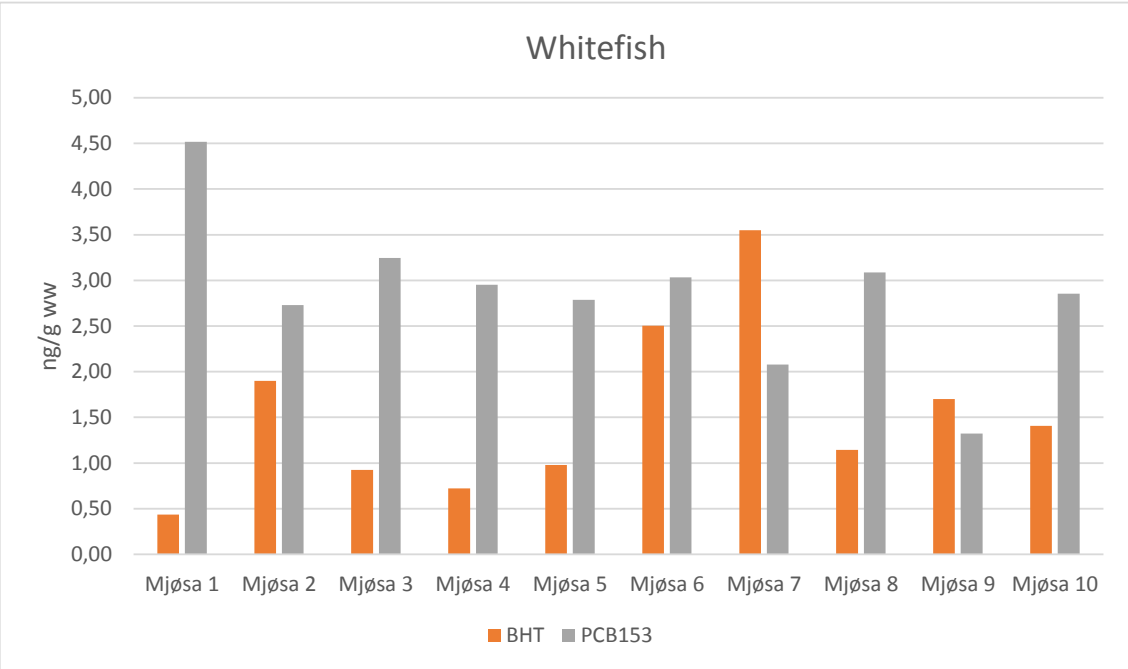


Figure 21: Concentrations of selected PBT compounds in soft tissue samples of White fish from Lake Mjøsa.

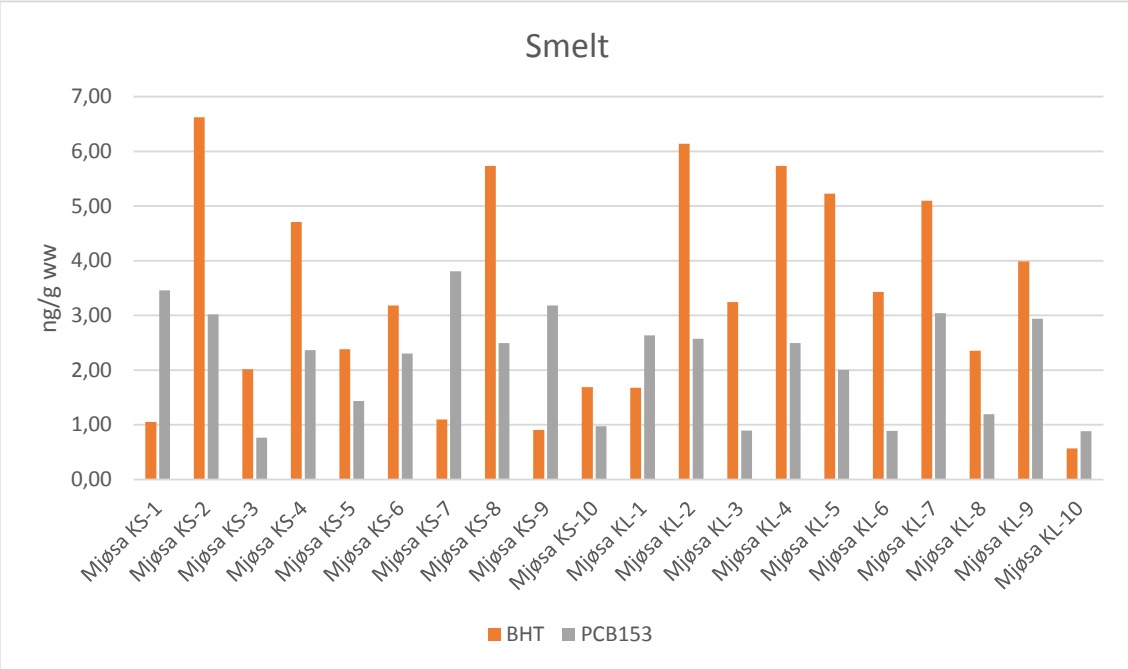


Figure 22: Concentrations of selected PBT compounds in soft tissue samples of smelt from Lake Mjøsa.

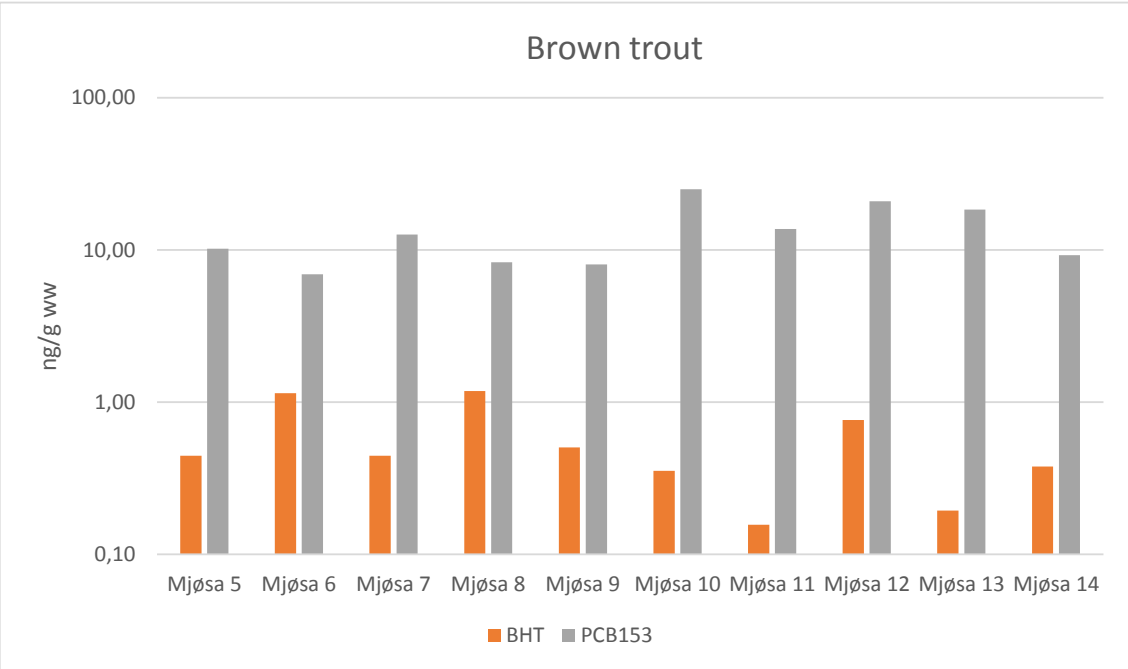


Figure 23: Logarithmic concentrations of selected PBT compounds in filet samples of brown trout from Lake Mjøsa.

3.5.2 Biomagnification of BHT and PCB153

The pairwise scatterplots between BHT and PCB153 concentrations (lipid weight) and isotopic ratios ($\delta^{15}N$ and $\delta^{13}C$) show that BHT seems to biodilute at higher trophic levels, whereas PCB153 biomagnifies (Figure 24). This is as observed in the biota samples from Oslofjord.

The scatterplot between N- and C-isotope ratios showed that hypopelagic zooplankton relied on a more ^{13}C-depleted food source than epipelagic zooplankton and the other organisms. This is a common phenomenon in deep oligotrophic lakes (Vander Zanden and Rasmussen, 1999), and a contributing factor to this may be due to algal uptake of respired CO_2 in the profundale zone (Rau 1978, 1980). Mysis, with its diurnal vertical migrations between the hypopelagic and epipelagic zones, had an intermediate $\delta^{13}C$ signature compared to the two zooplankton groups. A difference in the $\delta^{15}N$ signature of epipelagic and hypopelagic zooplankton can in part be attributed to the different species composition, with herbivorous clodocerans dominating in the epipelagic zone and more omnivorous copepods in the hypopelagic zone. Piscovorous brown trout and cannibalistic smelt are the top predators in this pelagic food web of Lake Mjøsa, and had subsequently the highest $\delta^{15}N$ values.

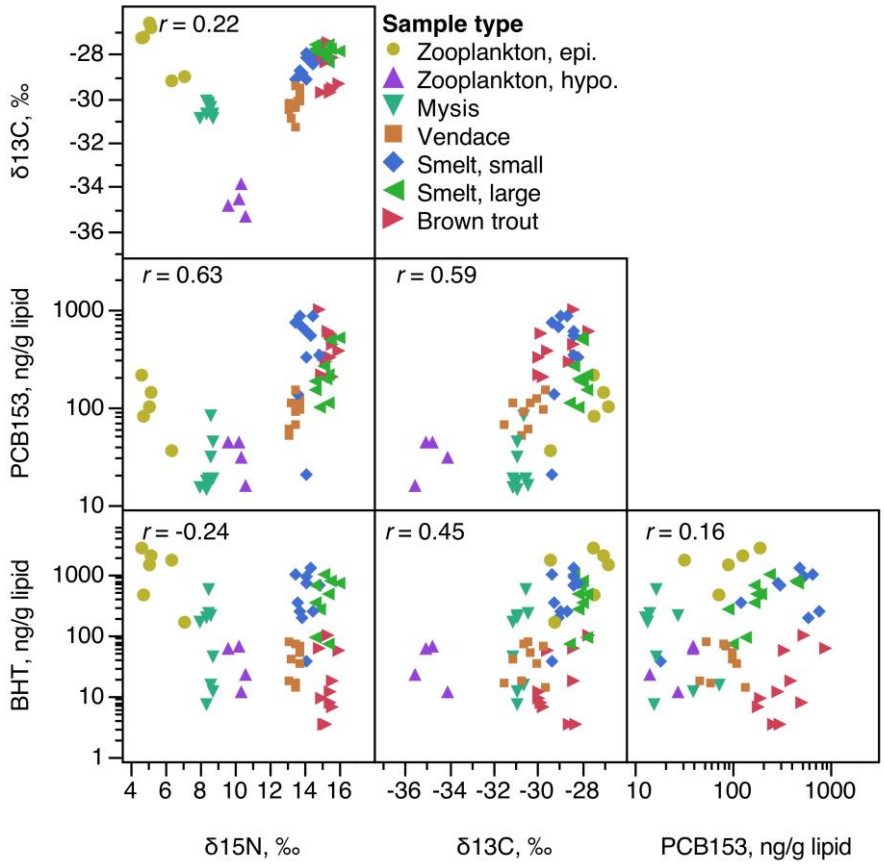


Figure 24: Scatterplot matrix of BHT and PCB153 concentrations (lipid weight) and N- and C-isotope ratios ($\delta^{15}N$ and $\delta^{13}C$) in biota samples from Lake Mjøsa. The pairwise correlation coefficient (Pearsons; log-transformed concentrations) is given within each plot.

We could not prove any statistical significant relationship between BHT concentrations and the N-isotope ratios in the pelagic food web of Lake Mjøsa, although a linear regression showed a week, although non-significant (p = 0.07), tendency for BHT to biodilute (Figure 25). Again, PCB153 biomagnified as expected. The TMFs for BHT and PCB153 in the Mjøsa food web were 0.65 and 2.16, respectively, though only the latter was statistically significant different from 1.

The epipelagic zooplankton samples had elevated BHT concentrations compared to hypopelagic zooplankton, Mysis and fish. It has been shown that BHT can be produced naturally in freshwater phytoplankton, both green algae and cyanobacteria (Babu and Wu, 2008). If this has occurred in Lake Mjøsa algae then it may have contributed to the elevated BHT concentrations in the epipelagic zooplankton samples, but so far we have no further evidence to support this view.

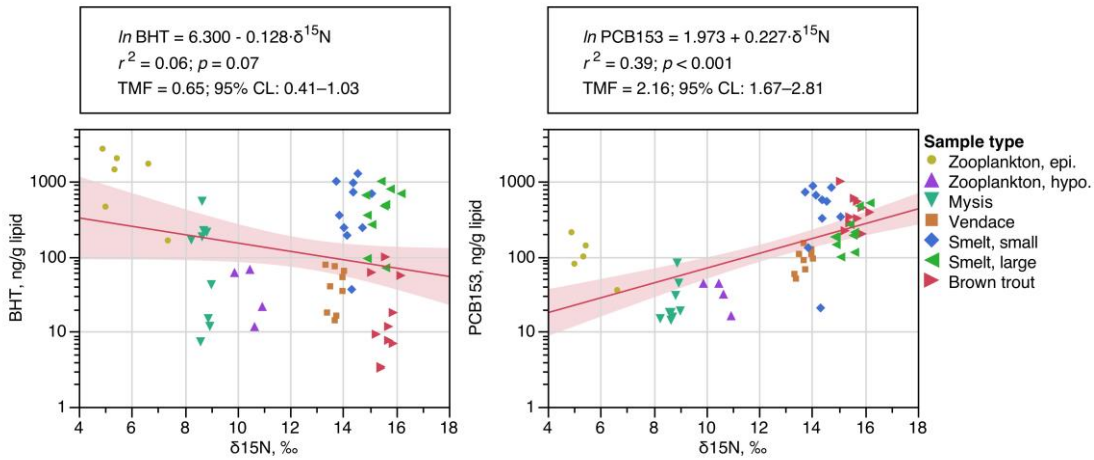


Figure 25: Linear regressions of BHT and PCB153 concentrations (lipid weight) on N-isotope ratios ($\delta^{15}N$) in biota samples from the pelagic food web of Lake Mjøsa. Regression statistics and trophic magnification factor (TMF) with 95% confidence limits (CL) are given above the plots.

3.5.3 Non-target screening

The Lake Mjøsa biota samples were also analysed by non-target analysis techniques. Confirmed, probable, and tentatively identified substances (Levels 1 to 3) in the Lake Mjøsa samples are listed in Apendix II. Presentation of the identified substances in the form of a venn diagram (Figure 26, data shown in Table 7), shows that 9 compounds are identified in all studied trophic levels of the Lake Mjøsa foodchain studied; 1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one, hexachlorobiphenyl, stearic acid, monoester with glycerol, buprenorphin, 1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethylnaphthalen-2yl]ethan-1-one (OTNE), dodecylphenol, p,p'-DDE, p,p'-DDT, nitrophenylhydrazine. A further 3 compounds, 4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone, 3-(5,5,6-trimethylbicyclo, were found in all levels of the foodchain apart from brown trout. This is likely to be due to the increased complexity of the brown trout liver sample matrix that resulted in fewer identifications and caution should be taken when extrapolating this to whether these compounds bioaccumulate or not.

Similarly to Oslofjord, known bioaccumulative contaminants hexachlorobiphenyl (PCB congeners 128-169), p,p´-DDE and p,p´-DDT were detetcted in all samples. The remaining compounds identified were only done so to level 3 and further confirmation of these is required before any further detail on their occurrence can be discussed.

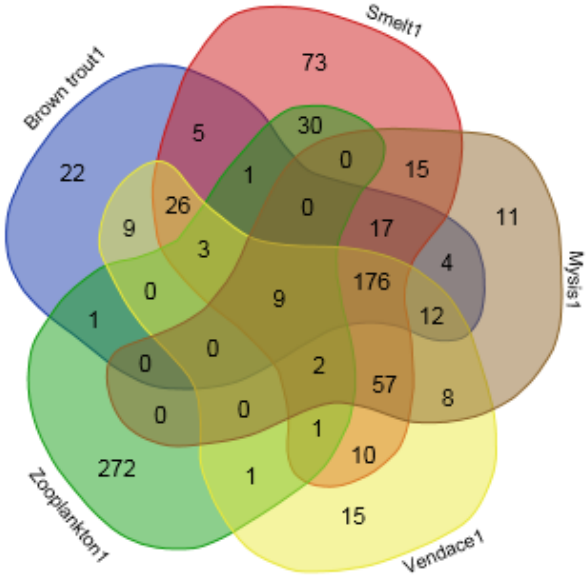


Figure 26: Venn diagram showing all compounds (ID level 1 to 3) found in the different sample matrices from Lake Mjøsa (calculated and drawn with online software by bioinformatics.psb.ugent.be).

Table 7: Summary of non-target screening results by occurrence in the Lake Mjøsa foodchain.
ID level in parenthesis

Matrices	No. of level 1-3 compounds	Level 1 and level 2 compound names
Brown trout, Mysis, Smelt, Vendace, Zooplankton	9	Hexachlorobiphenyl (1), p,p'-DDE (1), p,p'-DDT (1),
Mysis, Smelt, Vendace, Zooplankton	2	
Brown trout, Smelt, Vendace, Zooplankton	3	Diethyl phthalate (2),
Brown trout, Mysis, Smelt, Vendace	176	
Smelt, Vendace, Zooplankton	1	
Brown trout, Smelt, Zooplankton	1	
Mysis, Smelt, Vendace	57	
Brown trout, Mysis, Vendace	12	
Brown trout, Mysis, Smelt	17	
Brown trout, Smelt, Vendace	26	Tri(2-chloroethyl) phosphate (1), Galaxolide (1),

The heatmap visualizing the Lake Mjøsa data clearly shows a different pattern to that of Oslofjord. As with Oslofjord the majority of the identifcations are at level 3 (yellow), with very few level 1 identified compounds (red) occurring in all 5 levels of the selected Lake Mjøsa foodchain (Figure 27). The heatmap shows that more successful level 3 and above identifications were made in smelt and that there appears to be no clear trend as one moves up the food chain. This may again be associated with the complexity of different sample matrices resulting in comparatively fewer positive identifications. Again, it is clear is that

environmental samples from the Lake Mjøsa contain a large number of identifiable compounds.

Similarly, for Lake Mjøsa there is a need to increase the identification certainty of the level 3 substances identified in the entire foodchain before they can be proposed for inclusion in screening programmes. The compounds that should be considered are 1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one, stearic acid monoester with glycerol, buprenorphin, [1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethylnaphthalen-2yl]ethan-1-one (OTNE), and nitrophenylhydrazine. Other compounds occuring in 4 or more trophic levels should also be considered at a later stage.

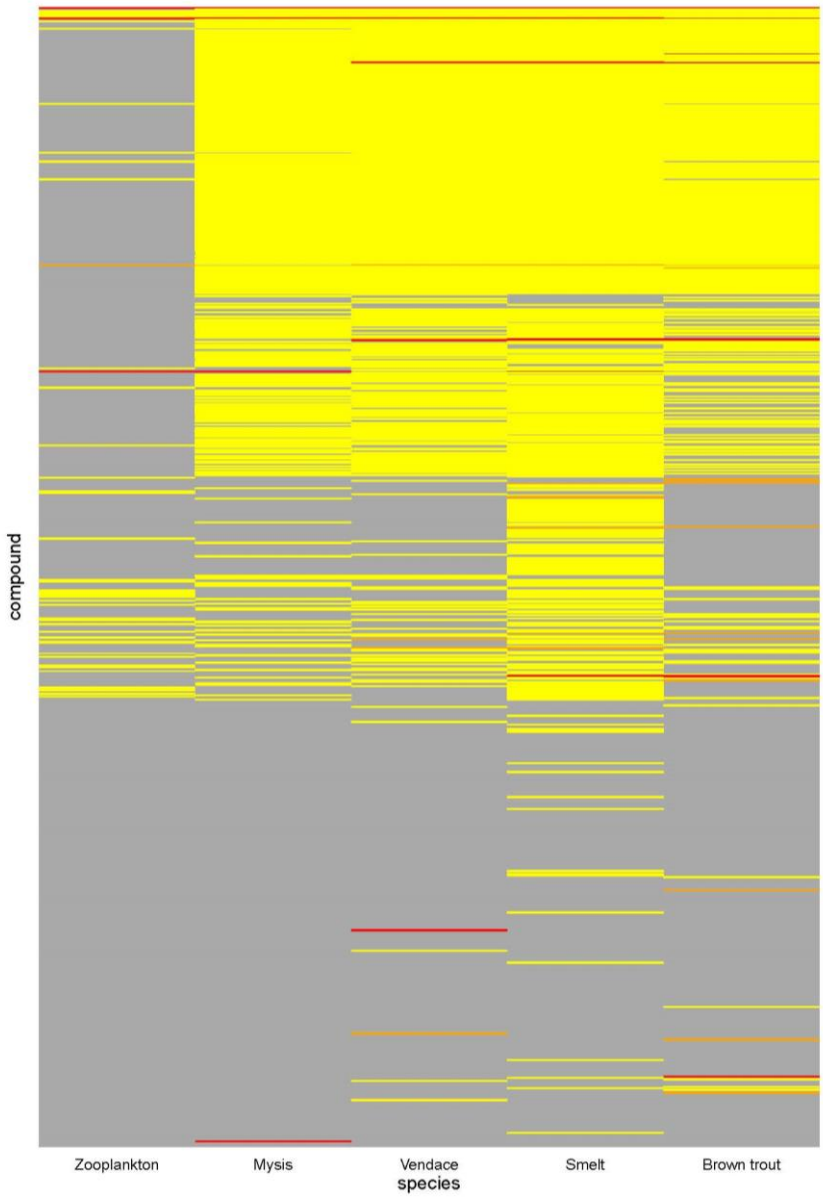


Figure 27: Heat map showing the compounds (Level 3 and above) identified in the Lake Mjøsa samples. Level 1= red, Level 2=orange, Level 3= yellow, Not found= grey).

3.1 Rat livers

3.1.1 Selected PBT compounds

Of the selected PBT substances, only BHT and PCB-153 were detected in rat liver samples from Oslo. The BHT concentrations were in the range of 0.5 – 13 ng/g fw. PCB-153 was in the range of 0.6 – 64 ng/g fw (Figure 28).

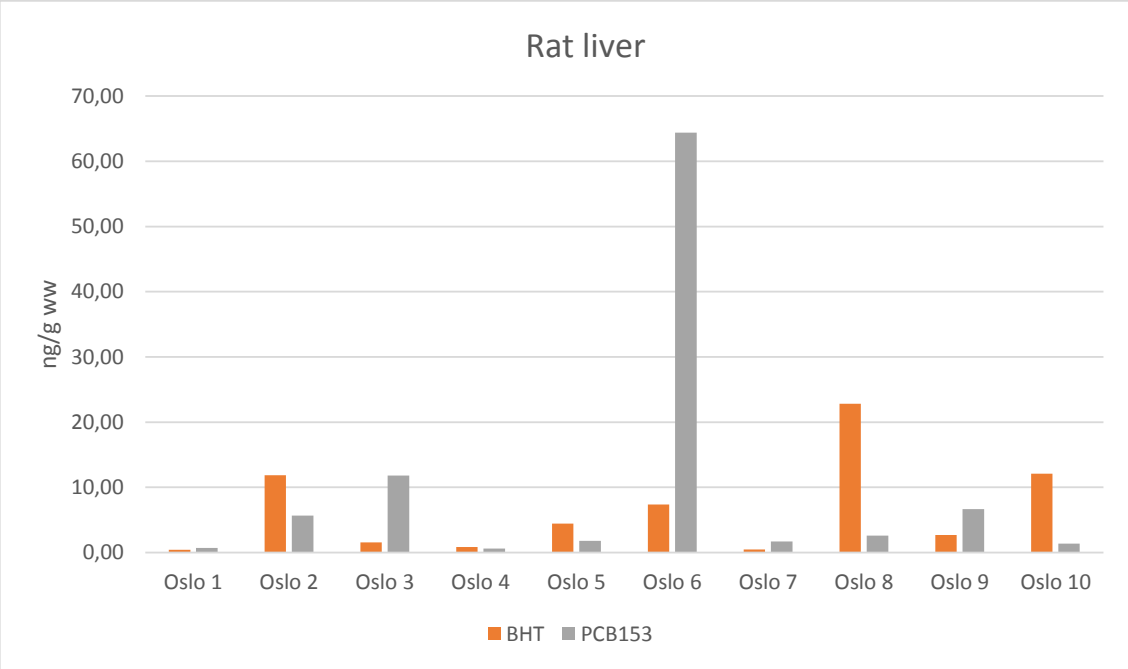


Figure 28: Concentrations of selected PBT compounds in liver samples of rats.

3.1.2 Non-target screening

Non-target screebing of the rat samples identified a number of anthropogenic substances in the livers of rats analysed, however the occurence of anthropogenic contaminants in rat livers is limited, potentially due to the high metabolic rates resulting in the rapid excretion of contaminants from their livers. Depite this rapid excretion, a number of compounds were identified to level 3. Benzophenone was the only level 1 identification, with diethyl phthalate, dibutyl phthalate, methyl hexadecyl ketone, isopropyl palmitate, elaidic acid, isopropyl ester , pentachlorobiphenyl, isopropyl stearate, octadecanoic acid, butyl ester and butyl myrisate identified to level 2. The palmitate, myristate and stearates derivatives are likely to be naturally occurring in the case of rats but due to their high use in personal care products, they have been included in this table (**Error! Reference source not found.**).

4. Environmental risk

An attempt was made to make a simple assessment of the environmental risk for each compound using the maximum and median measured environmental concentration (MEC) and dividing this by the published predicted no-effect concentration (PNEC), where available. This method of risk assessment will provide a general indication if there is any risk posed to the environment from the levels of an individual chemical. This evaluation does not rule out the risks associated with the combined effects of mixtures of chemicals, which may have a combined effect when present at concentrations below the PNEC.

4.1 Organic phosphites

None of the organic phosphites investigated in this screening study pose a direct threat to the environment, however it is not possible to eliminate any risks posed by any possible products resulting from the transformation of organic phosphites.

4.2 Selected PBT compounds

None of the detected PBT compounds (BHT and PBO) was present at concentrations in WWTW effluent at concentrations above the PNECs for receiving waters (BHT: $PNEC_{aqua}$ = 1.4 µg/L; PBO: 6 µg/L) (INCHEM, 2002, EPA, 2006) and therefore pose little direct risk. This PNEC is derived from a 21 day reproduction test with *Daphnia magna* using an assessment factor of 50. BHT was found to occur in all studied biota samples, however, a closer inspection revealed that BHT seems to biodilute in contrast to for example PCB-153.

4.1 Compounds detected by non-target screening

The non-target screening methodology allowed for qualitative rather than quantitative determination therefore, a risk assessment is not possible at this stage.

5. Conclusions and further work

- The selected organic phosphites were absent from all of the samples analysed.
- WWTW effluent is a source of BHT and PBO and WWTV sludge is a source of BHT.
- Landfill leachate is a source of BHT.
- BHT was shown to accumulate in marine and freshwater sediments receiving treated wastewater.
- BHT were detected in Oslofjord and Lake Mjøsa biota, however, BHT seems to biodilute in contrast to for example PCB-153

- Neither BHT nor PBO were present in WWTW effluent at concentrations above the PNECs for receiving waters and therefore pose little direct risk. There might be a risk associated with the accumulation of BHT in sediments and biota, however, this have not been evaluated.
- Five compounds were identified in all levels of the Oslofjord foodchain studied; galaxolide, hexachlorobiphenyl, p,p´-DDE, PFOS and PFOSA. Tonalide and carbenoxolone were found in all levels of the Oslofjord foodchain apart from cod.
- Nine compounds were identified in all studied trophic levels of the Lake Mjøsa foodchain studied; 1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one, Hexachlorobiphenyl stearic acid, monoester with glycerol, buprenorphin, 1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethylnaphthalen-2yl]ethan-1-one (OTNE), dodecylphenol, p,p'-DDE, p,p'-DDT, nitrophenylhydrazine. A further 2 compounds, 4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone and 3-(5,5,6-Trimethylbicyclo, were found in all levels of the foodchain apart from brown trout.
- In rats, benzophenone was the only level 1 identification, with diethyl phthalate, dibutyl phthalate, methyl hexadecyl ketone, isopropyl palmitate, elaidic acid, isopropyl ester, pentachlorobiphenyl, isopropyl stearate, octadecanoic acid, butyl ester and butyl myrisate identified to level 2.
- For the results of this project to be able to inform future screening programmes the first step would be to increase the identification certainty of the high number of level 3 compounds (tenatative candidates) to at least level 2 (probable).

6. References

Babu, B., and Wu, J.-T. (2008) Production of Natural Butylated Hydroxytoluene as an Antioxidant by Freshwater Phytoplankton. Journal of Phycology 44(6): 1447–1454.
Benford, D., Ceccatelli, S., Cottrill, B., Dinovi, M., Dogliotti, E., Edler, L., Farmer, P., Furst, P., Hoogenboom, L., Knutsen, H.K., Haldorsen, A.-K.L., Metzler, M., Nebbia, C.S., O'keeffe, M., Rietjens, I., Schrenk, D., Silano, V., Van Loveren, H., Vleminckx, C., Wester, P., Bergman, A., Boobis, A., Cravedi, J.-P., Filipic, M., Johansson, N., Machala, M., Merletti, F., Papke, O., Van Leeuwen, R., Van Leeuwen, S., Macleod, M., Cioacata, G., Gustavsson, N. and Bordajandi, L.R. (2012) Scientific opinion on emerging and novel brominated flame retardants (BFRs) in food. EFSA J., 10, 2908, 2125 pp.
Borgå, K., Kidd, K.A., Muir, D.C., Berglund, O., Conder, J.M., Gobas, F.A., Kucklick, J., Malm, O., and Powell, D.E. 2011. Trophic magnification factors: Considerations of ecology, ecosystems, and study design. Integrated environmental assessment and management 8(1): 64–84.
Boonnorat, J., Chiemchaisri, C., Chiemchaisri, W. and Yamamoto, K. (2014) Removals of phenolic compounds and phthalic acid esters in landfill leachate by microbial sludge of two-stage membrane bioreactor. J. Hazard. Mater., 277, 93-101.
Elder, V.A., Proctor, B.L. and Hites, R.A. (1981) Organic compounds found near dump sites in Niagara Falls, New York. *Environ. Sci. Technol., 15*, 1237-1243.
EPA (2006) Reregistration Eligibility Decision (RED) Document for Piperonyl Butoxide (PBO). URL: http://www.epa.gov/pesticides/reregistration/REDs/piperonyl_red.pdf [Accessed 31.03.2015].
Fries, E. and Püttmann, W. (2004) Monitoring of the antioxidant BHT and its metabolite BHT-CHO in German river water and ground water. Sci. Total Environ., 319, 269-282.
Grigoriadou, A. and Schwarzbauer, J. (2011) Non-target Screening of Organic Contaminants in Sediments from the Industrial Coastal Area of Kavala City (NE Greece). Water Air Soil Pollut, 214, 623-643.
Inchem (2002) 2,6-DI-TERT-BUTYL-P-CRESOL (BHT). URL: http://www.inchem.org/documents/sids/sids/128370.pdf [Accessed 31.03.2015].
Kuramochi, H., Takigami, H., Scheringer, M. and Sakai, S.-I. (2014) Estimation of physicochemical properties of 52 non-PBDE brominated flame retardants and evaluation of their overall persistence and long-range transport potential. Sci. Total Environ., 491–492, 108-117.
Liu, R., Ruan, T., Song, S., Lin, Y. and Jiang, G. (2015) Determination of synthetic phenolic antioxidants and relative metabolites in sewage treatment plant and recipient river by high performance liquid chromatography–electrospray tandem mass spectrometry. J. Chromatogr. A, 1381, 13-21.
Lundebye, A.K., Hove, H., Måge, A., Bohne, V.J.B. and Hamre, K. (2010) Levels of synthetic antioxidants (ethoxyquin, butylated hydroxytoluene and butylated hydroxyanisole) in fish feed and commercially farmed fish. Food Additives & Contaminants: Part A, 27, 1652-1657.
Managaki, S., Kobayashi, T., Hondo, H., Miyake, A. and Masunaga, S. (2011) Substance flow analysis of HBCD, considering the switch to its alternatives. Organohalogen Compd., 73, 2063-2066, 2064 pp.
Rau, G. (1978) Carbon-13 depletion in a subalpine lake: carbon flow implications. Science 201: 901-902.
Rau, G. (1980) Carbon-13/carbon-12 variation in subalpine lake aquatic insects: food sources implications. Canadian Journal of Fisheries and Aquatic Sciences 37: 742-746.

Rodil, R., Quintana, J.B., Concha-Graña, E., López-Mahía, P., Muniategui-Lorenzo, S. and Prada-Rodríguez, D. (2012) Emerging pollutants in sewage, surface and drinking water in Galicia (NW Spain). Chemosphere, 86, 1040-1049.
Sekizawa, J. and Greenberg, M.M. (2001) Diphenylmethane diisocyanate (MDI). Concise Int. Chem. Assess. Doc., 27, i-iv, 1-32.
Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P. and Hollender, J. (2014) Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. Environ. Sci Tecnol.. 48, 2097-2098.
Schymanski, E.L., Singer, H.P., Jaroslav Slobodnik Ipolyi, I.M. et al. (2015) Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. Anal. Bioanl. Chem. 407, 6237-3255.
Vander Zanden, M.J. and Rasmussen, J.B. (1999) Primary consumer δ13C and δ15N and the trophic position of aquatic consumers. Ecology 80(4): 1395–1404.

Appendix I: Results of target analyses

Tables with all analytical results follow. Concentrations are given in ng/L (water), ng/g dry weight (sludge and sediment), and ng/g wet weight (biota).

Occurrence of phosphites in biota from Oslofjord, Mjøsa and rat livers (n=10 for each matrix).										
Sample Matrix	Phosphite Compound									
	CAS 3806-34-6	CAS 31570-04-4	CAS 25448-25-3	CAS 26523-78-4	CAS 101-02-0	CAS 26741-53-7	CAS 26544-23-0	CAS 77745-66-5	CAS 15647-08-2	CAS 25550-98-5
Krill	<20	<20	<20	<20	<20	<20	<20	<20	<20	<20
Northern Shrimp	<20	<20	<20	<20	<20	<20	<20	<20	<20	<20
Herring	<200	<20	<20	<20	<20	<20	<20	<20	<20	<20
Cod liver	<200	<40	<40	<40	<40	<40	<40	<40	<40	<40
Zooplankton	<20	<20	<20	<20	<20	<20	<20	<20	<20	<20
Mysis	<20	<20	<20	<20	<20	<20	<20	<20	<20	<20
Vendace	<100	<20	<20	<20	<20	<20	<20	<20	<20	<20
Smelt	<50	<20	<20	<20	<20	<20	<20	<20	<20	<20
Brown Trout	<100	<20	<20	<20	<20	<20	<20	<20	<20	<20
Rat Liver	<200	<40	<40	<40	<40	<40	<40	<40	<40	<40

Occurrence of phosphites in landfill effluent, WWTW effluent and sludge, and receiving sediments.										
Sample Matrix	Phosphite Compound									
	CAS 3806-34-6	CAS 31570-04-4	CAS 25448-25-3	CAS 26523-78-4	CAS 101-02-0	CAS 26741-53-7	CAS 26544-23-0	CAS 77745-66-5	CAS 15647-08-2	CAS 25550-98-5
ISI effluent (n=3)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
ISI effluent particulates (n=3)	<50	<50	<50	<50	<50	<50	<50	<50	<50	<50
Lindum effluent (n=3)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
Lindum effluent particulates (n=3)	<50	<50	<50	<50	<50	<50	<50	<50	<50	<50
VEAS effluent (n=5)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
VEAS sludge (n=5)	<50	<50	<50	<50	<50	<50	<50	<50	<50	<50
HIAS effluent (n=5)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
HIAS sludge (n=5)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
Tomasjord effluent (n=5)	<25	<500	<25	<25	<25	<25	<25	<25	<25	<25
Oslofjord sediment (n=5)	<50	<50	<50	<50	<50	<50	<50	<50	<50	<50
Mjøsa sediment (n=5)	<50	<50	<50	<50	<50	<50	<50	<50	<50	<50

Occurrence of PBT compounds in wastewater samples and leachate (concentrations in ng/L)								
Location	Matrices	BHT	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos- phate	MDI
Tomasjord	Effluent	523	< 6,91	221,35	< 2,55	< 2,27	< 1,50	< 5,00
Tomasjord	Effluent	1007	< 13,90	111,34	< 1,91	< 1,71	< 1,50	< 5,00
Tomasjord	Effluent	1053	< 14,76	70,27	< 0,54	< 0,93	< 1,50	< 5,00
Tomasjord	Effluent	891	< 27,72	82,10	< 1,60	< 1,13	< 1,50	< 5,00
Tomasjord	Effluent	1200	< 39,12	65,95	< 1,15	< 41,05	< 1,50	< 5,00
HIAS 1	Effluent	419	< 7,60	233,18	< 3,51	< 4,54	< 1,50	< 5,00
HIAS 2	Effluent	411	< 2,21	219,57	< 1,29	< 1,18	< 1,50	< 5,00
HIAS 3	Effluent	374	< 31,45	782,79	< 145	< 19,89	< 1,50	< 5,00
HIAS 4	Effluent	377	< 3,10	128,46	< 2,86	< 2,93	< 1,50	< 5,00
HIAS 5	Effluent	451	< 3,21	109,43	< 2,33	< 1,62	< 1,50	< 5,00
VEAS 1	Effluent	831	< 41,20	< 1,91	< 2,39	< 4,05	< 1,50	< 5,00
VEAS 2	Effluent	858	< 4,93	28,00	< 1,31	< 1,75	< 1,50	< 5,00
VEAS 3	Effluent	532	< 5,91	67,34	< 2,29	< 1,47	< 1,50	< 5,00
VEAS 4	Effluent	423	< 2,55	< 0,66	< 1,08	< 1,20	< 1,50	< 5,00
VEAS 5	Effluent	166	< 3,48	55,40	< 1,47	< 1,63	< 1,50	< 5,00
ISI 1	Leachate P	82	< 1,17	< 0,27	< 0,48	< 0,68	< 1,50	< 5,00
ISI 2	Leachate P	281	< 2,85	< 0,73	< 1,35	0,00	< 1,50	< 5,00
Lindum 1	Leachate P	213	< 10,08	< 3,71	< 6,52	0,00	< 1,50	< 5,00
Lindum 2	Leachate P	732	< 44,33	< 1,21	< 2,19	0,00	< 1,50	< 5,00
Lindum 3	Leachate P	376	< 9,95	< 1,43	< 2,30	< 5,27	< 1,50	< 5,00
ISI 1	Leachate W	200	< 4,25	< 2,31	< 3,70	< 2,11	< 1,50	< 5,00
ISI 2	Leachate W	1392	< 4,74	< 2,07	< 3,26	< 1,07	< 1,50	< 5,00
Lindum 2	Leachate W	371	< 4,07	< 1,32	< 2,00	< 1,38	< 1,50	< 5,00
Lindum 3	Leachate W	349	< 30,46	< 10,97	< 13,40	< 12,45	< 1,50	< 5,00

Occurrence of PBT compounds in sludge and sediments (concentrations in ng/g dry weight)								
Location	Matrices	BHT	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos- phate	MDI
HIAS 1	Sludge	812	1,77	< 5,34	< 10,28	< 18,06	< 7,28	< 1,50
HIAS 2	Sludge	635	1,54	< 11,42	< 3,78	< 5,01	< 2,70	< 1,50
HIAS 3	Sludge	672	1,43	< 10,95	< 5,14	< 13,20	< 1,69	< 1,50
HIAS 4	Sludge	556	1,40	< 3,31	< 3,73	< 12,55	< 0,63	< 1,50
HIAS 5	Sludge	625	1,61	< 4,39	< 15,37	< 17,48	< 1,20	< 1,50
VEAS 1	Sludge	97	1,44	< 100,51	< 3,67	< 12,34	< 0,86	< 1,50
VEAS 2	Sludge	122	1,10	< 4,45	< 1,79	< 6,01	< 0,40	< 1,50
VEAS 3	Sludge	186	1,23	< 2,49	< 13,92	< 26,42	< 1,34	< 1,50
VEAS 4	Sludge	173	1,24	< 4,19	< 10,26	< 19,35	< 0,52	< 1,50
VEAS 5	Sludge	100	1,79	< 104,96	< 7,77	< 5,08	< 0,69	< 1,50
Oslofjord 1	Sediment	56,29	0,28	< 0,68	< 0,16	< 0,87	< 3,21	< 1,50
Oslofjord 2	Sediment	101,78	0,27	< 0,46	< 0,14	< 0,80	< 2,62	< 1,50
Oslofjord 3	Sediment	22,22	0,20	< 0,33	< 0,15	< 0,87	< 2,59	< 1,50
Oslofjord 4	Sediment	39,03	0,32	< 1,78	< 0,32	< 1,99	< 4,00	< 1,50
Oslofjord 5	Sediment	37,85	< 0,38	< 0,69	< 0,31	< 1,86	< 3,81	< 1,50
Mjøsa 1	Sediment	17,91	0,28	< 0,44	< 0,07	< 0,14	< 0,30	< 1,50
Mjøsa 2	Sediment	32,93	0,16	< 0,53	< 0,08	< 0,17	< 0,33	< 1,50
Mjøsa 3	Sediment	88,18	0,26	< 0,78	< 0,12	< 0,19	< 0,30	< 1,50
Mjøsa 4	Sediment	20,41	< 0,06	< 0,50	< 0,08	< 0,14	< 0,29	< 1,50
Mjøsa 5	Sediment	93,95	0,20	< 1,18	< 0,19	< 0,35	< 0,44	< 1,50

Occurrence of PBT compounds in marine biota from Oslofjord (concentrations in ng/g fresh weight)								
Matrices	BHT	PCB153	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos- phate	MDI
Krill	0,63	2,51	< 0,05	< 0,01	< 0,01	< 0,02	< 1,50	< 5,00
Krill	1,01	3,78	< 0,21	< 0,02	< 0,04	< 0,05	< 1,50	< 5,00
Krill	3,35	3,21	< 0,08	< 0,03	< 0,03	< 0,05	< 1,50	< 5,00
Krill	8,29	3,25	< 0,16	< 0,05	< 0,04	< 0,05	< 1,50	< 5,00
Krill	5,27	2,62	< 0,12	< 0,05	< 0,04	< 0,08	< 1,50	< 5,00
Krill	9,89	3,45	< 0,11	< 0,03	0,04	< 0,07	< 1,50	< 5,00
Krill	3,15	3,14	< 0,12	< 0,01	< 0,02	< 0,04	< 1,50	< 5,00
Krill	1,68	3,01	< 0,13	< 0,04	< 0,05	< 0,06	< 1,50	< 5,00
Krill	0,82	3,87	< 0,08	< 0,01	< 0,02	< 0,04	< 1,50	< 5,00
Krill	3,02	2,44	< 0,06	< 0,01	< 0,02	< 0,03	< 1,50	< 5,00
Shrimps	0,53	2,10	< 0,03	< 0,04	< 0,10	< 0,06	< 1,50	< 5,00
Shrimps	0,87	3,10	< 0,03	< 0,01	< 0,03	< 0,03	< 1,50	< 5,00
Shrimps	0,42	2,38	< 0,07	< 0,05	< 0,03	< 0,03	< 1,50	< 5,00
Shrimps	0,95	2,34	< 0,03	< 0,01	< 0,01	< 0,02	< 1,50	< 5,00
Shrimps	0,43	2,32	< 0,06	< 0,03	< 0,06	< 0,03	< 1,50	< 5,00
Shrimps	2,39	2,61	< 0,04	< 0,01	< 0,02	< 0,02	< 1,50	< 5,00
Shrimps	0,49	2,63	< 0,09	< 0,25	< 0,73	< 0,06	< 1,50	< 5,00
Shrimps	1,08	2,33	< 0,03	< 0,02	< 0,03	< 0,03	< 1,50	< 5,00
Shrimps	0,52	2,85	< 0,08	< 0,04	< 0,08	< 0,10	< 1,50	< 5,00
Shrimps	1,43	2,60	< 0,93	< 0,01	< 0,02	< 0,06	< 1,50	< 5,00
Herring	3,15	56,03	< 0,20	< 0,78	< 1,53	< 0,13	< 1,50	< 5,00
Herring	1,68	53,62	< 0,11	< 0,05	< 0,07	< 0,07	< 1,50	< 5,00
Herring	4,26	12,98	< 0,08	< 0,01	< 0,02	< 0,06	< 1,50	< 5,00
Herring	3,81	86,51	< 0,11	< 0,03	< 0,05	< 0,05	< 1,50	< 5,00
Herring	2,26	24,42	< 0,32	< 0,59	< 1,16	< 0,13	< 1,50	< 5,00
Herring	0,45	37,57	< 0,09	< 0,02	< 0,02	< 0,05	< 1,50	< 5,00
Herring	1,58	20,20	< 0,24	< 0,19	< 0,37	< 0,46	< 1,50	< 5,00
Herring	1,22	28,40	< 0,27	< 0,10	< 0,13	0,09	< 1,50	< 5,00
Herring	0,81	47,58	< 0,08	< 0,02	< 0,02	< 0,03	< 1,50	< 5,00
Herring	1,77	44,79	< 0,33	< 0,15	< 0,22	< 0,18	< 1,50	< 5,00
Cod liver	4,12	885,32	< 2,50	< 0,59	< 1,02	< 1,59	< 1,50	< 5,00
Cod liver	8,73	890,90	< 0,55	< 0,33	< 0,63	< 19,73	< 1,50	< 5,00
Cod liver	7,03	748,45	< 2,52	< 1,00	< 0,92	< 2,02	< 1,50	< 5,00
Cod liver	2,21	601,05	< 0,59	< 0,28	< 0,55	< 0,41	< 1,50	< 5,00
Cod liver	7,71	662,53	< 0,64	< 1,49	< 1,46	< 1,61	< 1,50	< 5,00
Cod liver	7,17	825,13	< 3,62	< 1,27	< 2,30	< 2,35	< 1,50	< 5,00
Cod liver	3,84	1294,82	< 13,58	< 0,29	< 0,52	< 1,30	< 1,50	< 5,00
Cod liver	11,86	1149,71	< 8,07	< 0,92	< 1,32	< 4,25	< 1,50	< 5,00
Cod liver	0,53	1940,93	< 0,81	< 0,62	< 0,97	< 0,85	< 1,50	< 5,00
Cod liver	3,75	1713,09	< 1,02	< 0,17	< 0,33	< 0,24	< 1,50	< 5,00

Occurrence of PBT compounds in freshwater biota from Mjøsa (concentrations in ng/g fresh weight)								
Matrices	BHT	PCB153	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos -phate	MDI
Mysis	0,26	0,99	< 0,10	< 0,03	< 0,04	< 0,07	< 1,50	< 5,00
Mysis	0,99	0,44	< 0,11	< 0,05	< 0,08	< 0,07	< 1,50	< 5,00
Mysis	0,34	1,89	< 0,15	< 0,04	< 0,04	< 0,10	< 1,50	< 5,00
Mysis	4,46	0,64	< 0,38	< 0,20	< 0,13	< 0,26	< 1,50	< 5,00
Mysis	5,18	0,36	< 0,28	< 0,13	< 0,21	< 0,47	< 1,50	< 5,00
Mysis	4,78	0,37	< 0,39	< 0,10	< 0,14	< 0,62	< 1,50	< 5,00
Mysis	0,16	0,40	< 0,10	< 0,03	< 0,03	< 0,05	< 1,50	< 5,00
Mysis	12,5	0,42	< 0,33	< 0,14	< 0,18	< 0,80	< 1,50	< 5,00
Mysis	4,46	0,40	< 0,27	< 4,37	< 8,49	< 0,46	< 1,50	< 5,00
Zooplankton E	1,44	0,10	< 0,43	< 0,06	< 0,09	< 0,17	< 1,50	< 5,00
Zooplankton E	2,03	0,14	< 0,04	< 0,01	< 0,01	< 0,02	< 1,50	< 5,00
Zooplankton E	0,46	0,08	< 0,08	< 0,01	< 0,01	< 0,02	< 1,50	< 5,00
Zooplankton E	5,43	0,42	< 0,05	< 0,01	< 0,01	< 0,19	< 1,50	< 5,00
Zooplankton E	4,81	0,10	< 0,06	< 0,22	< 0,11	< 0,04	< 1,50	< 5,00
Zooplankton E	0,49	< 0,01	< 0,09	< 0,02	< 0,03	< 0,07	< 1,50	< 5,00
Zooplankton H	0,32	0,86	< 0,32	< 0,05	< 0,08	< 0,08	< 1,50	< 5,00
Zooplankton H	1,44	1,01	< 0,25	< 0,29	< 0,48	< 0,10	< 1,50	< 5,00
Zooplankton H	1,70	1,10	< 0,24	< 0,07	< 0,10	< 0,10	< 1,50	< 5,00
Zooplankton H	1,09	0,80	< 0,17	< 0,05	< 0,04	< 0,09	< 1,50	< 5,00
Whitefish	0,44	4,52	< 0,15	< 0,06	< 0,11	< 0,13	< 1,50	< 5,00
Whitefish	1,90	2,73	< 0,12	< 0,14	< 0,16	< 0,27	< 1,50	< 5,00
Whitefish	0,93	3,24	< 0,09	< 0,06	< 0,12	< 0,75	< 1,50	< 5,00
Whitefish	0,72	2,95	< 0,41	< 0,49	< 1,07	< 0,14	< 1,50	< 5,00
Whitefish	0,98	2,79	< 0,49	< 0,17	< 0,22	< 0,21	< 1,50	< 5,00
Whitefish	2,50	3,03	< 0,11	< 0,24	< 0,17	< 0,06	< 1,50	< 5,00
Whitefish	3,55	2,08	< 0,09	< 0,06	< 0,08	< 0,27	< 1,50	< 5,00
Whitefish	1,14	3,09	< 0,19	< 1,20	< 1,74	< 0,58	< 1,50	< 5,00
Whitefish	1,70	1,32	< 0,08	< 0,01	< 0,02	< 0,02	< 1,50	< 5,00
Whitefish	1,41	2,85	< 0,16	< 0,09	< 0,07	< 0,01	< 1,50	< 5,00
Smelt S	1,05	3,45	< 0,05	< 0,01	< 0,01	< 0,03	< 1,50	< 5,00
Smelt S	6,62	3,02	< 0,90	< 0,17	< 0,21	< 0,54	< 1,50	< 5,00
Smelt S	2,01	0,76	< 0,21	< 0,03	< 0,03	< 0,06	< 1,50	< 5,00
Smelt S	4,71	2,36	< 1,49	< 0,83	< 1,28	< 0,53	< 1,50	< 5,00
Smelt S	2,38	1,44	< 0,05	< 0,02	< 0,02	< 0,02	< 1,50	< 5,00
Smelt S	3,18	2,30	< 0,26	< 0,66	< 1,38	< 0,24	< 1,50	< 5,00
Smelt S	1,10	3,80	< 0,11	< 0,02	< 0,03	< 0,05	< 1,50	< 5,00
Smelt S	5,73	2,49	< 1,34	< 0,24	< 0,37	< 0,55	< 1,50	< 5,00
Smelt S	0,91	3,18	< 0,33	< 0,03	< 0,05	< 0,10	< 1,50	< 5,00
Smelt S	1,69	0,97	< 0,04	< 0,02	< 0,03	< 0,01	< 1,50	< 5,00
Smelt L	1,68	2,64	< 0,20	< 0,04	< 0,08	< 0,08	< 1,50	< 5,00
Smelt L	6,14	2,57	< 1,13	< 0,16	< 0,26	< 0,33	< 1,50	< 5,00
Smelt L	3,24	0,90	< 0,11	< 0,04	< 0,07	< 0,07	< 1,50	< 5,00

Occurrence of PBT compounds in freshwater biota from Mjøsa (concentrations in ng/g fresh weight)								
Matrices	BHT	PCB153	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos -phate	MDI
Smelt L	5,73	2,49	< 1,34	< 0,24	< 0,37	< 0,99	< 1,50	< 5,00
Smelt L	5,22	2,00	< 0,36	< 0,18	< 0,22	< 0,16	< 1,50	< 5,00
Smelt L	3,43	0,89	< 0,14	< 0,09	< 0,16	< 0,04	< 1,50	< 5,00
Smelt L	5,10	3,04	< 3,71	< 0,10	< 0,14	< 0,16	< 1,50	< 5,00
Smelt L	2,35	1,19	< 0,06	< 0,01	< 0,01	< 0,03	< 1,50	< 5,00
Smelt L	3,99	2,94	< 0,19	< 0,16	< 0,12	< 0,17	< 1,50	< 5,00
Smelt L	0,57	0,88	< 0,09	< 0,02	< 0,04	< 0,04	< 1,50	< 5,00
Brown trout	0,44	10,19	< 0,05	< 0,09	< 0,15	< 0,02	< 1,50	< 5,00
Brown trout	1,14	6,91	< 0,05	< 0,03	< 0,03	< 0,03	< 1,50	< 5,00
Brown trout	0,44	12,65	< 0,06	< 0,02	< 0,03	< 0,10	< 1,50	< 5,00
Brown trout	1,19	8,28	< 0,04	< 0,05	< 0,07	< 0,05	< 1,50	< 5,00
Brown trout	0,50	8,04	< 0,03	< 0,01	< 0,01	< 0,05	< 1,50	< 5,00
Brown trout	0,35	25,08	< 0,12	< 0,03	< 0,02	< 0,07	< 1,50	< 5,00
Brown trout	0,16	13,73	< 0,08	< 0,02	< 0,05	< 0,05	< 1,50	< 5,00
Brown trout	0,76	20,86	< 0,11	< 0,02	< 0,05	< 0,05	< 1,50	< 5,00
Brown trout	0,19	18,44	< 0,07	< 0,02	< 0,02	< 0,04	< 1,50	< 5,00
Brown trout	0,38	9,25	< 0,07	< 0,01	< 0,01	< 0,02	< 1,50	< 5,00

Occurrence of PBT compounds in rat liver from Oslo (concentrations in ng/g fresh weight)								
Matrices	BHT	PCB153	Dibenzyl -toluene	Butoxide	Cyanox	Octa- benzone	Bromphos -phate	MDI
Rat liver	0,45	0,70	< 0,14	< 0,03	< 0,05	< 0,09	< 1,50	< 5,00
Rat liver	11,85	5,67	< 1,36	< 0,22	< 0,25	< 0,47	< 1,50	< 5,00
Rat liver	1,57	11,81	< 0,40	< 0,10	< 0,14	< 0,18	< 1,50	< 5,00
Rat liver	0,87	0,62	< 0,19	< 0,06	< 0,08	< 0,10	< 1,50	< 5,00
Rat liver	4,44	1,79	< 0,84	< 0,34	< 0,37	< 0,56	< 1,50	< 5,00
Rat liver	7,38	64,38	< 0,62	< 0,13	< 0,17	< 0,33	< 1,50	< 5,00
Rat liver	0,49	1,71	< 0,18	< 0,07	< 0,09	< 0,09	< 1,50	< 5,00
Rat liver	22,81	2,60	< 0,67	< 0,28	< 0,26	< 0,49	< 1,50	< 5,00
Rat liver	2,70	6,65	< 0,55	< 0,10	< 0,13	< 0,22	< 1,50	< 5,00
Rat liver	12,08	1,39	< 0,70	< 0,21	< 0,27	< 0,97	< 1,50	< 5,00

Appendix II: Results of non-target analyses

Non-target screening results for GC-HRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
Krill	C13H10O	182,0732	119-61-9	Benzophenone	1
	C12H14O4	222,0892	84-66-2	Diethyl phthalate	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C17H34O2	270,2559	110-27-0	Isopropyl myristate	2
	C19H38O2	298,2872	143-91-6	Isopropyl palmitate	2
	C21H42O2	326,3185	112-10-7	Isopropyl stearate	2
	C30H50	410,3913	7683-64-9	Squalene	2
	C9H14O	138,1045	42747-41-1	2,5,5-Trimethylcyclohex-2-enone	3
	C10H18O2	170,1307	706-14-9	5-hexyldihydro-2(3H)-Furanone	3
	C14H14N2	210,1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210,1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H22O2	222,1620		Dimethylethyl-benzenediol	3
	C16H32	224,2504	629-73-2	1-Hexadecene	3
	C15H15NO	225,1154		N-(1-naphthyl)-cyclobutanecarboxamide,	3
	C19H40	268,3130		tetramethyl-pentadecane	3
	C17H24O3	276,1725	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
Northern Shrimp	C18H26O	258,1984	1222-05-5	Galaxolide	1
	C12H14O4	222,0892	84-66-2	Diethyl phthalate	2
	C15H15NO	225,1154		N-(1-naphthyl)-cyclobutanecarboxamide	2
	C16H24O	232,1827	10541-56-7	p-Octylacetophenone	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2

Non-target screening results for GC-HRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C30H50	410,3913	7683-64-9	Squalene	2
	C31H50O2	454,3811		3-Acetoxyurs-13-ene	2
Herring	C12H18O	178,1358		Trimethylcyclohexylidene propanone	3
	C14H14N2	210,1157		2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210,1157		2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210,1157		2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C18H26O	258,1984	1222-05-5	Galaxolide	1
	C14H8Cl4	315,9380		DDE	2
	C12H5Cl5	323,8834		Pentachlorobiphenyl	2
	C12H5Cl5	323,8834		Pentachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H3Cl7	391,8054		heptachlorobiphenyl	2
	C15H32	212,2504	629-62-9	Pentadecane	3
	C17H34	238,2661		Heptadecane	3
Cod liver	C13H10O	182,0732	119-61-9	Benzophenone	1
	C18H26O	258,1984	1222-05-5	Galaxolide	1
	C5H5N3O2	139,0382		Pyrazinecarboxamide, 3,4-dihydro-3-oxo-	2
	C12H14O4	222,0892	84-66-2	Diethyl phthalate	2
	C14H8Cl4	315,9380		DDE	2
	C12H5Cl5	323,8834		Pentachlorobiphenyl	2
	C12H5Cl5	323,8834		pentachlorobiphenyl	2
	C12H5Cl5	323,8834		pentachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2

Non-target screening results for GC-HRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H4Cl6	357,8444		hexachlorobiphenyl	2
	C12H3Cl7	391,8054		heptachlorobiphenyl	2
	C12H3Cl7	391,8054		heptachlorobiphenyl	2
	C12H3Cl7	391,8054		heptachlorobiphenyl	2
	C12H3Cl7	391,8054		heptachlorobiphenyl	2
	C12H2Cl8	425,7665		octachlorobiphenyl	2
	C12H2Cl8	425,7665		octachlorobiphenyl	2
	C12H16O	176,1201		Butylacetophenone	3
	C14H20O2	220,1462		Phenol, 2,5-bis(1-methylethyl)-, acetate	3
	C15H30O	226,2297		Pentadecanone	3
	C16H32O2	256,2402		Tetradecanoic acid, ethyl ester	3
	C16H22O4	278,1518		Benzenedicarboxylic acid, diisooctyl ester	3
	C18H34O2	282,2559		Ethyl 9-hexadecenoate	3
	C19H36O4	328,2614		Methyl 15-acetoxyhexadecanoate	3

Non-target screening results for GCxGC-LRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS No.	Compound name	ID level
Krill	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H10Cl4	318	53-19-0	o,p-DDD	1
	C14H10Cl4	318	72-54-8	p,p-DDD	1
	C14H9Cl5	364	104215-84-1	p,p'-DDT	1
	C12H4Cl6	370	74472-40-5	Hexachlorobiphenyl	1
	C10H6Cl8	406	57-74-9	Cis-Chlordane	2
	C10H5Cl9	440	39765-80-5	cis/trans-nonachlor	2
Northern shrimp	C6H5Cl2N	161	95-82-9	Benzenamine, 2,5-dichloro-	3

Non-target screening results for GCxGC-LRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS No.	Compound name	ID level
	C12H18N2O3S	270	64-77-7	Tolbutamide (or breakdown product)	3
	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C12H5Cl5	324	38380-01-7	Pentachlorobiphenyl	3
	C12H5Cl5	324	37680-73-2	Pentachlorobiphenyl	3
	C12H5Cl5	324	31508-00-6	Pentachlorobiphenyl	3
	C12H5Cl5	324	32598-14-4	Pentachlorobiphenyl	3
	C18H15O4P	326	115-86-6	Triphenyl phosphate	1
	C12H4Cl6	358	52663-72-6	Hexachlorobiphenyl	3
	C12H4Cl6	358	52712-04-6	Pentachlorobiphenyl	3
	C12H4Cl6	358	69782-90-7	Hexachlorobiphenyl	3
	C12H4Cl6	358	35065-28-2	Hexachlorobiphenyl	3
	C12H4Cl6	358	35065-28-2	Hexachlorobiphenyl	3
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
	C12H3Cl7	392	35065-29-3	Heptachlorobiphenyl	3
	C12H3Cl7	392	35065-29-3	Heptachlorobiphenyl	3
	C12H3Cl7	392	35065-29-3	Heptachlorobiphenyl	3
	C12H3Cl7	392	35065-29-3	Heptachlorobiphenyl	3
	C12H3Cl7	392	35065-29-3	Heptachlorobiphenyl	3
	C12H6Br4O	482	189084-61-5	Tetrabromodiphenyl ether	3
Herring	C18H26O	258	21145-77-7	Tonalide	3
	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H10Cl4	318	72-54-8	p,p-DDD	1
	C9H18Cl3O4P	326	13674-84-5	Tris(2-chloropropyl)phosphate	1
	C18H15O4P	326	115-86-6	Triphenyl phosphate	1
	C14H10Cl4	330	104215-84-1	p,p'-DDT	1
	C12H4Cl6	358	35065-28-2	Hexachlorobiphenyl	1
	C12H8Cl6O	378	60-57-1	Dieldrin	2
	C12H8Cl6O	378	60-57-1	Dieldrin	2
	C10H5Cl7O	386	1024-57-3	Heptachlor exo epoxide	2
	C10H6Cl8	406	5103-71-9	Cis-chlordane	2
	C10H6Cl8	406	5103-74-2	Cis-Chlordane	2
	C10H5Cl9	440	39765-80-5	cis/trans-Nonachlor	2
	C10H5Cl9	491	39765-80-5	trans-Nonachlor	2
	C10H5Cl9	491	5103-73-1	cis/trans-Nonachlor	2
Cod liver	C15H24O	220	128-37-0	BHT	2

Non-target screening results for GCxGC-LRToF analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS No.	Compound name	ID level
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H10Cl4	318	72-54-8	p,p'-DDD	1
	C12H4Cl6	358	52712-04-6	Hexachlorobiphenyl	1
	C12H8Cl6O	378	60-57-1	Dieldrin	2
	C10H5Cl9	440	39765-80-5	trans-Nonachlor	2
	C10H5Cl9	440	5103-73-1	cis-Nonachlor	2
	C10H5Cl9	440	3734-49-4	4,7-Methano-1H-indene, 1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-	2
	C10H5Cl9	440	39765-80-5	trans-Nonachlor	2
	C12Cl10	494	2051-24-3	Decachlorobiphenyl	1
	C10Cl12	540	2385-85-5	Mirex	1

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
Krill	C9H16N4OS	229,1117		tebuthiuron	1
	C18H35NO2	298,2742		spiroxamine	1
	C20H26O2	299,2012		norethynodrel	1
	C16H15F2N3Si	316,1069		flusilazole	1
	C11H15NO2	194,1184		isoprocarb	2
	C25H24F6N4	495,1981		hydramethylnon	2
	C3H9N	59,0735	75-50-3	trimethylamine	3
	C3H9N	59,0735	107-10-8	propylamine	3
	C4H9N	71,0735	123-75-1	pyrrolidine	3
	C3H7NO2	89,0477	625-51-4	N-(hydroxymethyl)acetamide	3
	C3H7NO2	89,0477	79-46-9	2-nitropropane	3
	C3H7NO2	89,0477	107-95-9	ß-alanine	3
	C3H7NO2	89,0477	108-03-2	1-nitropropane	3
	C3H7NO2	89,0477	107-97-1	sarcosine	3
	C3H7NO2	89,0477	56-41-7	L-alanine	3
	C6H7N	93,0578	62-53-3	Aniline	3
	C6H7N	93,0578	108-99-6	3-methylpyridine	3
	C6H7N	94,0653		maybe aniline, phenylamine or methylpyridine	3
	C5H10O2	102,0681	75-98-9	pivalic acid	3
	C5H10O2	102,0681	108-21-4	isopropyl acetate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C5H10O2	102,0681	109-52-4	valeric acid	3
	C5H10O2	102,0681	109-60-4	propyl acetate	3
	C5H10O2	102,0681	505-65-7	1,3-dioxepane	3
	C5H10O2	102,0681	97-99-4	tetrahydrofurfuryl alcohol	3
	C5H10O2	102,0681	116-53-0	2-methylbutyric acid	3
	C5H10O2	102,0681	503-74-2	isovaleric acid	3
	C5H13NO	103,0997	3179-63-3	3-dimethylaminopropan-1-ol	3
	C5H13NO	103,0997	108-16-7	1-(dimethylamino)propan-2-ol	3
	C5H13NO	103,0997	6291-85-6	3-ethoxypropylamine	3
	C8H14	110,1096	931-87-3	(Z)-cyclooctene	3
	C8H14	110,1096	3710-30-3	octa-1,7-diene	3
	C4H5N3O	111,0433	71-30-7	cytosine	3
	C5H9NO2	115,0633	4394-85-8	N-Formylmorpholine	3
	C5H9NO2	115,0633	147-85-3	L-proline	3
	C5H9NO2	115,0633	923-02-4	N-(hydroxymethyl)methacrylamide	3
	C5H9NO2	115,0633	14205-39-1	methyl 3-aminocrotonate	3
	C4H8O4	120,0423	19757-97-2	Methyl hydroxymethoxyacetate	3
	C8H8O	120,0575	96-09-3	(epoxyethyl)benzene	3
	C8H8O	120,0575	98-86-2	acetophenone	3
	C9H12	120,0939	98-82-8	Isopropylbenzol	3
	C9H12	120,0939	95-63-6	1,2,4-trimethylbenzene	3
	C9H12	120,0939	108-67-8	mesitylene	3
	C9H12	120,0939	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3
	C9H12	120,0939	3048-64-4	5-vinylnorborn-2-ene	3
	C2H7NO3S	125,0147	107-35-7	taurine	3
	C7H14N2	126,1157	5351-04-2	3-diethylaminopropiononitrile	3
	C5H8N2O2	128,0586	77-71-4		3
	C6H13NO2	131,0946	61-90-5	L-leucine	3
	C6H13NO2	131,0946	622-40-2	2-morpholinoethanol	3
	C10H12	132,0939	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3
	C10H12	132,0939	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	C10H12	132,0939	768-56-9	4-phenylbut-1-ene	3
	C9H10O	134,0732	93-55-0	propiophenone	3
	C9H10O	134,0732	104-54-1	cinnamyl alcohol	3
	C10H14	134,1096	95-93-2		3
	C10H14	134,1096	527-53-7		3
	C10H14	134,1096	99-87-6	p-cymene	3
	C10H14	134,1096	4488-57-7	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C10H14	134,1096	25340-17-4	diethylbenzene	3
	C10H14	134,1096	68411-44-9	Benzene, butyl-, branched and linear	3
	C10H14	134,1096	105-05-5	1,4-diethylbenzene	3
	C5H5N5	135,0545	73-24-5	adenine	3
	C7H13NO2	143,0946	7747-35-5	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	3
	C7H13NO2	143,0946	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	C2H6ClO3P	143,9743	16672-87-0	Ethephon	3
	C6H13NOS	147,0718	141-98-0	O-isopropyl ethylthiocarbamate	3
	C8H4O3	148,016	85-44-9	phthalic anhydride	3
	C5H4N4O2	152,0334	69-89-6	xanthine	3
	C5H4N4O2	152,0334	2465-59-0	oxypurinol	3
	C8H12N2O	152,095	2814-20-2	G27550	3
	C6H7N3O2	154,0611	86490-48-4	nitrophenylhydrazine	3
	C7H5NS	158,0031		benzothiazole	3
	C10H10N2	158,0844	2243-62-1	1,5-naphthylenediamine	3
	C10H10N2	158,0844	479-27-6	1,8-naphthylenediamine	3
	C12H14	158,1096	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	C12H14	158,1096	3748-13-8	m-bis(1-methylvinyl)benzene	3
	C7H15NO3	161,1052	541-15-1	Levocarnitin	3
	C6H19NSi2	161,1056	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	C9H6O3	162,0317	93-35-6	7-hydroxycoumarine	3
	C12H18	162,1409	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	C12H18	162,1409	7397-06-0		3
	C12H18	162,1409	4904-61-4	cyclododeca-1,5,9-triene	3
	C12H18	162,1409	99-62-7	1,3-diisopropylbenzene	3
	C12H18	162,1409	100-18-5	1,4-diisopropylbenzene	3
	C12H18	162,1409	25321-09-9	diisopropylbenzene	3
	C9H8O3	164,0473	156-06-9	phenylpyruvic acid	3
	C9H8O3	164,0473	15206-55-0	methyl benzoylformate	3
	C11H16O	164,1201	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	C11H16O	164,1201	88-60-8	6-tert-butyl-m-cresol	3
	C11H16O	164,1201	2409-55-4	2-tert-butyl-p-cresol	3
	C11H16O	164,1201	583-03-9	fenipentol	3
	C9H11NO2	165,079	94-09-7	benzocaine	3
	C9H11NO2	165,079	51-66-1	methacetin	3
	C9H11NO2	165,079	1129-41-5	Metolcarb	3
	C9H11NO2	165,079	938-73-8	Ethenzamide	3
	C9H11NO2	165,079	18595-18-1	Benzoic acid, 3-amino-4-methyl-, methyl ester	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C9H11NO2	165,079	24461-61-8	methyl (R)-aminophenylacetate	3
	C9H10O3	166,063	120-47-8	ethyl 4-hydroxybenzoate	3
	C9H10O3	166,063	121-32-4	ethyl vanillin	3
	C9H10O3	166,063	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	C9H10O3	166,063	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3
	C9H10O3	166,063	11070-44-3	tetrahydromethylphthalic anhydride	3
	C9H10O3	166,063	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	C9H10O3	166,063	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	C6H14O5	166,0841	59113-36-9	oxybispropanediol	3
	C9H14O3	170,0943	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	C9H14O3	170,0943	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	C6H17NO3Si	179,0978	13822-56-5	3-(trimethoxysilyl)propylamine	3
	C9H8O4	180,0423	50-78-2	acetylsalicyl acid	3
	C13H10O	182,0732	3218-36-8	p-phenylbenzaldehyde	3
	C13H10O	183,0809		benzophenone	3
	C14H20	188,1565	81-03-8		3
	C14H20	188,1565	1203-17-4	1,1,2,3,3-pentamethylindan	3
	C11H15NO2	193,1103	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	C11H15NO2	193,1103	2631-40-5	Isoprocarb	3
	C11H15NO2	193,1103	2686-99-9	3,4,5-Trimethacarb	3
	C11H15NO2	193,1103	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	C11H15NO2	193,1103	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	C11H14O3	194,0943	94-26-8	Butyl 4-hydroxybenzoate	3
	C11H14O3	194,0943	4247-02-3	isobutyl 4-hydroxybenzoate	3
	C11H14O3	194,0943	614-45-9	tert-butyl perbenzoate	3
	C12H22O2	198,162	88-41-5		3
	C12H22O2	198,162	111-81-9	methyl undec-10-enoate	3
	C12H22O2	198,162	688-84-6	2-ethylhexyl methacrylate	3
	C12H22O2	198,162	51000-52-3	vinyl neodecanoate	3
	C12H22O2	198,162		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	C12H22O2	198,162	89-48-5	menthyl acetate	3
	C12H22O2	198,162	150-84-5	citronellyl acetate	3
	C12H22O2	198,162	713-95-1	dodecan-5-olide	3
	C12H22O2	198,162	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	C12H22O2	198,162	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	C12H11NO2	202,0858		carbaryl	3
	C8H21NOSi2	203,1162	10416-59-8	trimethylsilyl N-	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
				trimethylsilylacetamidate	
	C13H16O2	204,115	947-19-3	Methanone, Irgacure 184	3
	C13H16O2	204,115	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	C13H16O2	204,115	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	C14H20O	204,1514	80-54-6	Bucinal	3
	C14H20O	204,1514	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	C13H18O2	206,1307	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	C14H8O2	208,0524	84-65-1	anthrachinone	3
	C14H8O2	208,0524	635-12-1	Anthracen-1,4-dione	3
	C8H19O4P	210,1021		Di-tert-butyl hydrogen phosphate	3
	C14H26O	210,1984		Degradation-Product	3
	C14H26O	210,1984	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	C16H26	218,2035	68648-87-3		3
	C14H20O2	220,1463	719-22-2	2,6-Di-tert-butylquinone	3
	C13H25NO2	227,1885		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	C15H22O2	234,162	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	C15H22O2	234,162	5444-75-7	2-ethylhexyl benzoate	3
	C16H26O	234,1984	54464-57-2	OTNE	3
	C16H26O	234,1984	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	C16H26O	234,1984	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	C16H26O	234,1984		Degradation-Product	3
	C16H26O	234,1984	68155-66-8		3
	C16H26O	234,1984	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	C16H26O	234,1984	121158-58-5	Phenol, dodecyl-, branched	3
	C15H24O2	236,1776	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	C13H15NO2	240,1		pyracarbolid	3
	C17H20O	240,1514	15087-24-8	3-benzylidenecamphor	3
	C16H35N	241,277	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	C16H35N	241,277	112-75-4	dimethyl(tetradecyl)amine	3
	C16H35N	241,277	1120-48-5	dioctylamine	3
	C10H14N2O5	242,0903	3424-98-4	Telbivudine	3
	C10H14N2O5	242,0903	50-89-5	thymidine	3
	C18H26	242,2035	1087-02-1	p-Dicyclohexylbenzene	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C12H24N2O3	244,1787	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	C16H22O2	246,162		Degradation-Product	3
	C18H30	246,2348	2719-62-2	6-Phenyldodecane	3
	C18H30	246,2348	25265-78-5	tetrapropylenebenzene	3
	C6H20N2O6S	248,1042	5080-22-8	N-isopropylhydroxylamine	3
	C14H16O4	248,1049	5292-53-5	diethyl (phenylmethylene)malonate	3
	C15H20O3	248,1412	71617-10-2	isopentyl p-methoxycinnamate	3
	C16H24O2	248,1776	18017-73-7	10-Phenyldecanoic acid	3
	C16H24O2	248,1776	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	C16H26O2	250,1933		Degradation-Product	3
	C16H26O2	250,1933	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	C16H26O2	250,1933	79-74-3	2,5-di-tert-pentylhydroquinone	3
	C16H28O2	252,2089	30507-70-1	(Z,E)-tetradeca-9,12-dienyl acetate	3
	C16H31NO	253,2406	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	C16H31NO	253,2406	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	C16H30O2	254,2246	142-90-5	dodecyl methacrylate	3
	C18H26O	258,1984	1222-05-5	Galaxolide	3
	C18H26O	258,1984	1506-02-1	Tonalide	3
	C18H26O	258,1984	68140-48-7	ATII (Traseolide)	3
	C14H12O3S	260,0507	33005-95-7	tiaprofenic acid	3
	C18H30O	262,2297	5892-47-7	2,4,6-tri-sec-butylphenol	3
	C15H23NO3	265,1678	6452-71-7	oxprenolol	3
	C12H26O4S	266,1552		dodecyl sulfuric acid	3
	C12H26O4S	266,1552		2-butyloctyl-sulfonic acid	3
	C12H27O4P	266,1647	126-73-8	tributyl phosphate	3
	C12H27O4P	266,1647	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	C16H26O3	266,1882	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	C16H26O3	266,1882	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	C18H34O	266,261		Degradation-Product	3
	C10H13N5O4	267,0968	58-61-7	adenosine	3
	C10H13N5O4	267,0968	30516-87-1	Zidovudine	3
	C14H22N2O3	267,1724		atenolol	3
	C17H32O2	268,2402	21643-42-5	tetradecyl acrylate	3
	C18H39N	269,3083	112-69-6	hexadecyldimethylamine	3
	C18H39N	269,3083	124-30-1	octadecylamine	3
	C9H13ClN6O2	272,0789	42471-28-3	nimustine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C18H24O2	272,1776	50-28-2	17-beta-Estradiol	3
	C18H24O2	272,1776	57-91-0	alfatradiol	3
	C18H26O2	274,1933	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	C18H26O2	274,1933	434-22-0	nandrolone	3
	C17H24O3	276,1725	456-59-7	cyclandelate	3
	C17H24O3	276,1725	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	C14H32O3Si	276,2121	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	3
	C14H32O3Si	276,2121	2943-75-1	triethoxyoctylsilane	3
	C16H22O4	278,1518	84-74-2	Dibutyl phthalate	3
	C16H22O4	278,1518	84-69-5	diisobutyl phthalate	3
	C16H22O4	278,1518	1962-75-0	dibutyl terephthalate	3
	C18H30O2	278,2246		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	C18H30O2	278,2246	506-26-3	gamolenic acid	3
	C18H32O2	280,2402	60-33-3	linoleic acid	3
	C18H35NO	281,2719	1593-77-7	Dodemorph	3
	C18H34O2	282,2559	112-80-1	Oleic acid	3
	C18H34O2	282,2559	2549-53-3	tetradecyl methacrylate	3
	C18H37NO	283,2875	124-26-5	stearamide	3
	C20H28O	284,214	52-76-6	lynestrenol	3
	C17H32O3	284,2351		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	C19H26O2	286,1933	63-05-8	Androstendion	3
	C19H26O2	286,1933	846-48-0	boldenone	3
	C16H30O4	286,2144	6846-50-0	TXIB	3
	C16H30O4	286,2144	7491-02-3	diisopropyl sebacate	3
	C20H30O	286,2297	3772-55-2		3
	C20H30O	286,2297	68-26-8	retinol	3
	C18H26O3	290,1882	5466-77-3	Ethylhexyl methoxycinnamate	3
	C20H34O	290,261	26266-77-3		3
	C18H28O3	292,2038	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	C20H36O	292,2766	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	C18H30O3	294,2195	2315-61-9	4-Octylphenol di-ethoxylate	3
	C21H28N	294,2216	57982-78-2	budipine	3
	C18H35NO2	297,2668	118134-30-8	Spiroxamine	3
	C20H26O2	298,1933	68-22-4	Norethisteron	3
	C18H34O3	298,2508	13040-19-2	diricinoleate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C18H21NO3	299,1521	125-29-1	Hydrocodone	3
	C18H21NO3	299,1521	76-57-3	codeine	3
	C18H21NO3	299,1521	968-46-7	deanol benzilate	3
	C20H31NO	301,2406	144-11-6	trihexyphenidyl	3
	C19H26O3	302,1882	584-79-2	(RS)-3-allyl-2-methyl-4-oxocyclopent-2-enyl-(1RS,3RS;1RS,3SR)-2,2-dimethyl-3-(2-methylprop-1-enyl)-cyclopropanecarboxylate (all isomers; ratio: 1:1:1:1:1:1:1:1)	3
	C19H26O3	302,1882	560-62-3	Androst-4-ene-3,17-dione, 9-hydroxy-	3
	C19H26O3	302,1882	566-48-3	formestane	3
	C20H30O2	302,2246	58-18-4	17-alpha-Methyltestosterone	3
	C20H30O2	302,2246	153-00-4	metenolone	3
	C17H34O4	302,2457	6731-36-8	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	3
	C20H32O2	304,2402	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	C20H32O2	304,2402	1424-00-6	mesterolone	3
	C19H32O3	308,2351	20427-84-3	4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group)	3
	C19H35NO2	309,2668	77-19-0	dicyclomine	3
	C22H30O	310,2297	54024-22-5	Desogestrel	3
	C19H34O3	310,2508	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	C19H23ClN2	314,155	303-49-1	clomipramine	3
	C21H30O2	314,2246	13956-29-1	cannabidiol	3
	C21H30O2	314,2246	1972-08-3	delta(9)-tetrahydrocannabinol	3
	C21H30O2	314,2246	57-83-0	Progesteron	3
	C21H30O2	314,2246	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	C18H34O4	314,2457	109-43-3	dibutyl sebacate	3
	C18H34O4	314,2457	110-33-8	dihexyl adipate	3
	C18H34O4	314,2457	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	C18H34O4	314,2457	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	C18H34O4	314,2457	871-70-5	1,18-octadecanedioic acid	3
	C20H28O3	316,2038	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	C20H28O3	316,2038	2137-18-0	gestonorone	3
	C20H32O3	320,2351		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3
	C17H36O3S	320,2385	111360-16-8	2-hexyldecyl mesylate	3
	C18H35AlO3	326,2402	13419-15-3	(octadecanoato-O)oxoaluminium	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C20H41NO2	327,3137	111-57-9	N-(2-hydroxyethyl)stearamide	3
	C22H32O2	328,2402	127-47-9	retinyl acetate	3
	C19H36O4	328,2614	56519-71-2	propane-1,3-diyl dioctanoate	3
	C20H26O4	330,1831	84-61-7	dicyclohexyl phthalate	3
	C24H42	330,3287	4445-07-2	octadecylbenzene	3
	C18H24ClN3O	333,1608	119168-77-3	Tebufenpyrad	3
	C18H24ClN3O	333,1608	125225-28-7	Ipconazole	3
	C20H31NO3	333,2304	77-23-6	carbetapentane	3
	C16FH19N4O3	334,1441	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	C18H26ClN3O	335,1764	118-42-3	Hydroxychloroquine	3
	C20H30O4	335,2205		dihexylphthalate or bis(4-methyl-2-pentyl)phthalate	3
	C17H36O6	336,2512	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	C22H43NO	337,3345		docos-13-enamide, Amides, C22 (unsaturated)	3
	C20H34O4	338,2457	25155-25-3		3
	C20H34O4	338,2457	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	C22H28O3	340,2038	51-98-9	Norethisterone acetate	3
	C22H28O3	340,2038	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	C22H28O3	340,2038	976-71-6	canrenone	3
	C24H23NO	342,1852	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	C22H30O3	342,2195	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	C22H30O3	342,2195	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	C23H34O2	342,2559	7069-42-3	retinyl propionate	3
	C20H38O4	342,277	762-12-9	bisdecanoyl peroxide	3
	C20H38O4	342,277	2915-57-3	bis(2-ethylhexyl) succinate	3
	C19H38N2O3	342,2882	4292-10-8	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	3
	C22H32O3	344,2351	434-05-9	Metenolone acetate	3
	C22H32O3	344,2351	520-85-4	Medroxyprogesteron	3
	C22H32O3	344,2351	2668-66-8	medrysone	3
	C20H22O2Si2	350,1158		Degradation-Product	3
	C20H32O5	352,225	363-24-6	dinoprostone	3
	C20H32O5	352,225	35121-78-9	epoprostenol	3
	C21H39NO3	353,293	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C20H26N4O2	354,2056	3811-75-4	Hexamidine	3
	C22H28NO3	354,2064	125-51-9	pipenzolate	3
	C16H34O6S	354,2076		2-(2-dodecyloxyethoxy)ethyl sulfonic acid	3
	C22H42O3	354,3134		(3S,4S)-3-hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone	3
	C21H40O4	356,2927	28510-23-8	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	3
	C21H40O4	356,2927	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	C21H42O4	358,3083	31566-31-1	stearic acid, monoester with glycerol	3
	C22H33NO3	359,246	139-62-8	cyclomethycaine	3
	C15H21Cl2FN2O3	366,0913	81406-37-3	Fluroxypyr-meptyl	3
	C24H30O3	366,2195	67392-87-4	drospirenone	3
	C22H42O4	370,3083	103-23-1	bis(2-ethylhexyl) adipate	3
	C22H42O4	370,3083	1330-86-5	diisooctyl adipate	3
	C22H28O5	372,1937	24916-90-3	9?,11?-epoxy-17,21-dihydroxy-16?-methylpregna-1,4-diene-3,20-dione	3
	C22H28O5	372,1937	599-33-7	prednylidene	3
	C22H30O5	374,2093	1172-63-0	Jasmolin II	3
	C22H30O5	374,2093	83-43-2	Methylprednisolone	3
	C22H26O6	386,1729	2618-77-1		3
	C22H28O6	388,1886	76-78-8	Quassin	3
	C23H24N4O2	388,1899		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	C24H38O4	390,277	117-84-0	Di-n-octylphthalate (DOP)	3
	C24H38O4	390,277	117-81-7	DEHP	3
	C24H38O4	390,277	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	C24H38O4	390,277	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	C25H30NO3	392,222	10405-02-4	Trospium	3
	C24H40O4	392,2927	474-25-9	chenodeoxycholic acid	3
	C24H40O4	392,2927	128-13-2	ursodeoxycholic acid	3
	C18H26FN3O4S	399,1628		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	C27H44O2	400,3341	41294-56-8	alphacalcidol	3
	C20H34O8	402,2254	77-90-7	Tributylacetylcitrate	3
	C23H20N2O3S	404,1195	57-96-5	sulfinpyrazone	3
	C22H28F2O5	410,1905	2135-17-3	flumetasone	3
	C22H28F2O5	410,1905	2557-49-5	diflorasone	3
	C25H48O4	412,3553	103-24-2	bis(2-ethylhexyl) azelate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C24H30O6	414,2042	107724-20-9	eplerenone	3
	C24H30O6	414,2042		2,6-bis(4-ethylphenyl)perhydro-1,3,5,7-tetraoxanaphth-4-ylethane-1,2-diol	3
	C25H37NO4	415,2723	155206-00-1	Bimatoprost	3
	C25H37NO4	415,2723	89365-50-4	Salmeterol	3
	C26H42O4	418,3083	28553-12-0	Diisononyl phthalate (DINP)	3
	C29H41NO4	467,3036	52485-79-7	Buprenorphin	3
	C30H37NO4	475,2723	126784-99-4	Ulipristal acetate	3
	BC21H45O12	499,304	30989-05-0	tris[2-[2-(2-methoxyethoxy)ethoxy]ethyl] orthoborate	3
	C32H39NO4	501,2879	83799-24-0	fexofenadine	3
	C30H53N3O6	551,3934	173334-57-1	aliskiren	3
	C30H46NO7P	563,3012	98048-97-6	Fosinopril	3
	C34H50O7	570,3557	5697-56-3	carbenoxolone	3
	C48H69N3O6	783,5186	27676-62-6		3
Northern Shrimp	C3H9N	59,0735	107-10-8	propylamine	3
	C4H9N	71,0735	123-75-1	pyrrolidine	3
	C3H7NO2	89,0477	625-51-4	N-(hydroxymethyl)acetamide	3
	C3H7NO2	89,0477	107-95-9	ß-alanine	3
	C3H7NO2	89,0477	107-97-1	sarcosine	3
	C3H7NO2	89,0477	56-41-7	L-alanine	3
	C6H7N	93,0578	62-53-3	Aniline	3
	C6H7N	93,0578	108-99-6	3-methylpyridine	3
	C5H10O2	102,0681	75-98-9	pivalic acid	3
	C5H10O2	102,0681	108-21-4	isopropyl acetate	3
	C5H10O2	102,0681	109-52-4	valeric acid	3
	C5H10O2	102,0681	109-60-4	propyl acetate	3
	C5H10O2	102,0681	505-65-7	1,3-dioxepane	3
	C5H10O2	102,0681	97-99-4	tetrahydrofurfuryl alcohol	3
	C5H10O2	102,0681	116-53-0	2-methylbutyric acid	3
	C5H10O2	102,0681	503-74-2	isovaleric acid	3
	C8H14	110,1096	931-87-3	(Z)-cyclooctene	3
	C8H14	110,1096	3710-30-3	octa-1,7-diene	3
	C4H5N3O	111,0433	71-30-7	cytosine	3
	C4H4N2O2	112,0273	123-33-1	Pyridazine-3,6-diol	3
	C4H4N2O2	112,0273	1193-24-4	6-hydroxy-1H-pyrimidin-4-one	3
	C5H9NO2	115,0633	4394-85-8	N-Formylmorpholine	3
	C5H9NO2	115,0633	147-85-3	L-proline	3
	C5H9NO2	115,0633	923-02-4	N-(hydroxymethyl)methacrylamide	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C5H9NO2	115,0633	14205-39-1	methyl 3-aminocrotonate	3
	C4H8O4	120,0423	19757-97-2	Methyl hydroxymethoxyacetate	3
	C8H8O	120,0575	96-09-3	(epoxyethyl)benzene	3
	C8H8O	120,0575	98-86-2	acetophenone	3
	C2H7NO3S	125,0147	107-35-7	taurine	3
	C5H6N2O2	126,0429	4866-00-6	4-methyloxazole-5-carboxamide	3
	C7H14N2	126,1157	5351-04-2	3-diethylaminopropiononitrile	3
	C5H8N2O2	128,0586	77-71-4		3
	C10H12	132,0939	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3
	C10H12	132,0939	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	C10H12	132,0939	768-56-9	4-phenylbut-1-ene	3
	C9H10O	134,0732	93-55-0	propiophenone	3
	C9H10O	134,0732	104-54-1	cinnamyl alcohol	3
	C2H6ClO3P	143,9743	16672-87-0	Ethephon	3
	C6H13NOS	147,0718	141-98-0	O-isopropyl ethylthiocarbamate	3
	C8H4O3	148,016	85-44-9	phthalic anhydride	3
	C9H8O2	148,0524	621-82-9	cinnamic acid	3
	C5H4N4O2	152,0334	69-89-6	xanthine	3
	C5H4N4O2	152,0334	2465-59-0	oxypurinol	3
	C6H7N3O2	154,0611	86490-48-4	nitrophenylhydrazine	3
	C2H11N2O4P	158,0456		1,2-ethanediamine	3
	C12H14	158,1096	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	C12H14	158,1096	3748-13-8	m-bis(1-methylvinyl)benzene	3
	C7H15NO3	161,1052	541-15-1	Levocarnitin	3
	C6H19NSi2	161,1056	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	C9H6O3	162,0317	93-35-6	7-hydroxycoumarine	3
	C12H18	162,1409	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	C12H18	162,1409	7397-06-0		3
	C12H18	162,1409	4904-61-4	cyclododeca-1,5,9-triene	3
	C12H18	162,1409	99-62-7	1,3-diisopropylbenzene	3
	C12H18	162,1409	100-18-5	1,4-diisopropylbenzene	3
	C12H18	162,1409	25321-09-9	diisopropylbenzene	3
	C9H8O3	164,0473	156-06-9	phenylpyruvic acid	3
	C9H8O3	164,0473	15206-55-0	methyl benzoylformate	3
	C11H16O	164,1201	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	C11H16O	164,1201	88-60-8	6-tert-butyl-m-cresol	3
	C11H16O	164,1201	2409-55-4	2-tert-butyl-p-cresol	3
	C11H16O	164,1201	583-03-9	fenipentol	3
	C9H10O3	166,063	120-47-8	ethyl 4-hydroxybenzoate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C9H10O3	166,063	121-32-4	ethyl vanillin	3
	C9H10O3	166,063	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	C9H10O3	166,063	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3
	C9H10O3	166,063	11070-44-3	tetrahydromethylphthalic anhydride	3
	C9H10O3	166,063	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	C9H10O3	166,063	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	C9H14O3	170,0943	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	C9H14O3	170,0943	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	C6H17NO3Si	179,0978	13822-56-5	3-(trimethoxysilyl)propylamine	3
	C9H8O4	180,0423	50-78-2	acetylsalicyl acid	3
	C13H10O	182,0732	119-61-9	benzophenone	3
	C13H10O	182,0732	3218-36-8	p-phenylbenzaldehyde	3
	C14H20	188,1565	81-03-8		3
	C14H20	188,1565	1203-17-4	1,1,2,3,3-pentamethylindan	3
	C13H18O	190,1358	125109-85-5	ß-methyl-3-(1-methylethyl)benzenepropanal	3
	C13H18O	190,1358	103-95-7	3-p-cumenyl-2-methylpropionaldehyde	3
	C13H18O	190,1358	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	3
	C11H15NO2	193,1103	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	C11H15NO2	193,1103	94-25-7	butamben	3
	C11H15NO2	193,1103	42542-10-9	3,4-methylenedioxymethamphetamine	3
	C11H15NO2	193,1103	1795-96-6	phenylalanine, ethyl ester	3
	C11H15NO2	193,1103	7298-73-9	N-Methylphenacetine	3
	C11H15NO2	193,1103	2631-40-5	Isoprocarb	3
	C11H15NO2	193,1103	2686-99-9	3,4,5-Trimethacarb	3
	C11H15NO2	193,1103	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	C11H15NO2	193,1103	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	C11H14O3	194,0943	94-26-8	Butyl 4-hydroxybenzoate	3
	C11H14O3	194,0943	4247-02-3	isobutyl 4-hydroxybenzoate	3
	C11H14O3	194,0943	614-45-9	tert-butyl perbenzoate	3
	C12H22O2	198,162	88-41-5		3
	C12H22O2	198,162	111-81-9	methyl undec-10-enoate	3
	C12H22O2	198,162	688-84-6	2-ethylhexyl methacrylate	3
	C12H22O2	198,162	51000-52-3	vinyl neodecanoate	3
	C12H22O2	198,162		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	C12H22O2	198,162	89-48-5	menthyl acetate	3
	C12H22O2	198,162	150-84-5	citronellyl acetate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C12H22O2	198,162	713-95-1	dodecan-5-olide	3
	C12H22O2	198,162	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	C12H22O2	198,162	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	C8H21NOSi2	203,1162	10416-59-8	trimethylsilyl N-trimethylsilylacetamidate	3
	C13H16O2	204,115	947-19-3	Methanone, Irgacure 184	3
	C13H16O2	204,115	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	C13H16O2	204,115	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	C14H20O	204,1514	80-54-6	Bucinal	3
	C14H20O	204,1514	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	C13H18O2	206,1307	15687-27-1	Ibuprofen	3
	C13H18O2	206,1307	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	C8H19O4P	210,1021		Di-tert-butyl hydrogen phosphate	3
	C14H26O	210,1984		Degradation-Product	3
	C14H26O	210,1984	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	C10H16N2O3	212,1161	125-40-6	secbutabarbital	3
	C10H16N2O3	212,1161	77-28-1	butobarbital	3
	C16H26	218,2035	68648-87-3		3
	C14H20O2	220,1463	719-22-2	2,6-Di-tert-butylquinone	3
	C4H6N4O3S2	222,995		acetazolamide	2
	C13H25NO2	227,1885		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	C15H22O2	234,162	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	C15H22O2	234,162	5444-75-7	2-ethylhexyl benzoate	3
	C16H26O	234,1984	54464-57-2	OTNE	3
	C16H26O	234,1984	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	C16H26O	234,1984	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	C16H26O	234,1984		Degradation-Product	3
	C16H26O	234,1984	68155-66-8		3
	C16H26O	234,1984	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	C16H26O	234,1984	121158-58-5	Phenol, dodecyl-, branched	3
	C15H24O2	236,1776	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	C16H35N	241,277	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	C16H35N	241,277	112-75-4	dimethyl(tetradecyl)amine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C16H35N	241,277	1120-48-5	dioctylamine	3
	C10H14N2O5	242,0903	3424-98-4	Telbivudine	3
	C10H14N2O5	242,0903	50-89-5	thymidine	3
	C18H26	242,2035	1087-02-1	p-Dicyclohexylbenzene	3
	C9H13N3O5	243,0855	147-94-4	cytarabine	3
	C12H24N2O3	244,1787	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	C16H22O2	246,162		Degradation-Product	3
	C18H30	246,2348	2719-62-2	6-Phenyldodecane	3
	C18H30	246,2348	25265-78-5	tetrapropylenebenzene	3
	C6H20N2O6S	248,1042	5080-22-8	N-isopropylhydroxylamine	3
	C14H16O4	248,1049	5292-53-5	diethyl (phenylmethylene)malonate	3
	C16H24O2	248,1776	18017-73-7	10-Phenyldecanoic acid	3
	C16H24O2	248,1776	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	C16H26O2	250,1933		Degradation-Product	3
	C16H26O2	250,1933	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	C16H26O2	250,1933	79-74-3	2,5-di-tert-pentylhydroquinone	3
	C16H28O2	252,2089	30507-70-1	(Z,E)-tetradeca-9,12-dienyl acetate	3
	C16H31NO	253,2406	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	C16H31NO	253,2406	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	C16H30O2	254,2246	142-90-5	dodecyl methacrylate	3
	C18H26O	258,1984	1222-05-5	Galaxolide	3
	C18H26O	258,1984	1506-02-1	Tonalide	3
	C18H26O	258,1984	68140-48-7	ATII (Traseolide)	3
	C14H12O3S	260,0507	33005-95-7	tiaprofenic acid	3
	C17H24O2	260,1776		Degradation-Product	3
	C18H30O	262,2297	5892-47-7	2,4,6-tri-sec-butylphenol	3
	C12H26O4S	266,1552		dodecyl sulfuric acid	3
	C12H26O4S	266,1552		2-butyloctyl-sulfonic acid	3
	C12H27O4P	266,1647	126-73-8	tributyl phosphate	3
	C12H27O4P	266,1647	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	C16H26O3	266,1882	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	C16H26O3	266,1882	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	C10H13N5O4	267,0968	58-61-7	adenosine	3
	C10H13N5O4	267,0968	30516-87-1	Zidovudine	3
	C17H32O2	268,2402	21643-42-5	tetradecyl acrylate	3
	C18H39N	269,3083	112-69-6	hexadecyldimethylamine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C18H39N	269,3083	124-30-1	octadecylamine	3
	C9H13ClN6O2	272,0789	42471-28-3	nimustine	3
	C18H24O2	272,1776	50-28-2	17-beta-Estradiol	3
	C18H24O2	272,1776	57-91-0	alfatradiol	3
	C18H26O2	274,1933	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	C18H26O2	274,1933	434-22-0	nandrolone	3
	C17H24O3	276,1725	456-59-7	cyclandelate	3
	C17H24O3	276,1725	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	C14H32O3Si	276,2121	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	3
	C14H32O3Si	276,2121	2943-75-1	triethoxyoctylsilane	3
	C19H21N2	277,1699	524-81-2	mebhydroline	3
	C16H22O4	278,1518	84-74-2	Dibutyl phthalate	3
	C16H22O4	278,1518	84-69-5	diisobutyl phthalate	3
	C16H22O4	278,1518	1962-75-0	dibutyl terephthalate	3
	C17H26O3	278,1882	3115-49-9	4-nonylphenoxy acetic acid (NPE1C)	3
	C18H30O2	278,2246		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	C18H30O2	278,2246	506-26-3	gamolenic acid	3
	C18H32O2	280,2402	60-33-3	linoleic acid	3
	C18H35NO	281,2719	1593-77-7	Dodemorph	3
	C18H34O2	282,2559	112-80-1	Oleic acid	3
	C18H34O2	282,2559	2549-53-3	tetradecyl methacrylate	3
	C18H37NO	283,2875	124-26-5	stearamide	3
	C20H28O	284,214	52-76-6	lynestrenol	3
	C17H32O3	284,2351		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	C19H26O2	286,1933	63-05-8	Androstendion	3
	C19H26O2	286,1933	846-48-0	boldenone	3
	C16H30O4	286,2144	6846-50-0	TXIB	3
	C16H30O4	286,2144	7491-02-3	diisopropyl sebacate	3
	C19H28O2	288,2089	481-30-1	Epitestosterone	3
	C19H28O2	288,2089	58-22-0	Testosterone	3
	C19H28O2	288,2089	53-43-0	prasterone	3
	C19H28O2	288,2089	1091-93-6	3-methoxyestra-2,5(10)-dien-17?-ol	3
	C18H26O3	290,1882	5466-77-3	Ethylhexyl methoxycinnamate	3
	C19H30O2	290,2246	521-18-6	androstanolone	3
	C20H34O	290,261	26266-77-3		3
	C18H28O3	292,2038	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C20H36O	292,2766	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	C18H30O3	294,2195	2315-61-9	4-Octylphenol di-ethoxylate	3
	C21H28N	294,2216	57982-78-2	budipine	3
	C18H35NO2	297,2668	118134-30-8	Spiroxamine	3
	C20H26O2	298,1933	68-22-4	Norethisteron	3
	C18H34O3	298,2508	13040-19-2	diricinoleate	3
	C18H21NO3	299,1521	125-29-1	Hydrocodone	3
	C18H21NO3	299,1521	76-57-3	codeine	3
	C18H21NO3	299,1521	968-46-7	deanol benzilate	3
	C18H36O3	300,2664	106-14-9	12-hydroxystearic acid	3
	C20H31NO	301,2406	144-11-6	trihexyphenidyl	3
	C20H30O2	302,2246	58-18-4	17-alpha-Methyltestosterone	3
	C20H30O2	302,2246	153-00-4	metenolone	3
	C17H34O4	302,2457	6731-36-8	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	3
	C20H32O2	304,2402	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	C20H32O2	304,2402	1424-00-6	mesterolone	3
	C19H32O3	308,2351	20427-84-3	4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group)	3
	C19H35NO2	309,2668	77-19-0	dicyclomine	3
	C22H30O	310,2297	54024-22-5	Desogestrel	3
	C19H34O3	310,2508	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	C19H23ClN2	314,155	303-49-1	clomipramine	3
	C21H30O2	314,2246	13956-29-1	cannabidiol	3
	C21H30O2	314,2246	1972-08-3	delta(9)-tetrahydrocannabinol	3
	C21H30O2	314,2246	57-83-0	Progesteron	3
	C21H30O2	314,2246	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	C18H34O4	314,2457	109-43-3	dibutyl sebacate	3
	C18H34O4	314,2457	110-33-8	dihexyl adipate	3
	C18H34O4	314,2457	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	C18H34O4	314,2457	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	C18H34O4	314,2457	871-70-5	1,18-octadecanedioic acid	3
	C20H28O3	316,2038	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	C20H28O3	316,2038	2137-18-0	gestonorone	3
	C20H32O3	320,2351		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C17H36O3S	320,2385	111360-16-8	2-hexyldecyl mesylate	3
	C19H30O4	322,2144	106807-78-7	2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C)	3
	C20H41NO2	327,3137	111-57-9	N-(2-hydroxyethyl)stearamide	3
	C22H32O2	328,2402	127-47-9	retinyl acetate	3
	C19H36O4	328,2614	56519-71-2	propane-1,3-diyl dioctanoate	3
	C20H26O4	330,1831	84-61-7	dicyclohexyl phthalate	3
	C24H42	330,3287	4445-07-2	octadecylbenzene	3
	C18H24ClN3O	333,1608	119168-77-3	Tebufenpyrad	3
	C18H24ClN3O	333,1608	125225-28-7	Ipconazole	3
	C20H31NO3	333,2304	77-23-6	carbetapentane	3
	C16FH19N4O3	334,1441	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	C17H36O6	336,2512	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	C22H43NO	337,3345		docos-13-enamide, Amides, C22 (unsaturated)	3
	C22H26O3	338,1882	10453-86-8	Resmethrin	3
	C20H34O4	338,2457	25155-25-3		3
	C20H34O4	338,2457	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	C19H24N4O2	340,1899	100-33-4	Pentamidine	3
	C21H26NO3	340,1907	53-46-3	Methanthelinium	3
	C22H28O3	340,2038	51-98-9	Norethisterone acetate	3
	C22H28O3	340,2038	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	C22H28O3	340,2038	976-71-6	canrenone	3
	C21H26O4	342,1831	96609-16-4	lifibrol	3
	C24H23NO	342,1852	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	C22H30O3	342,2195	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	C22H30O3	342,2195	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	C23H34O2	342,2559	7069-42-3	retinyl propionate	3
	C20H38O4	342,277	762-12-9	bisdecanoyl peroxide	3
	C20H38O4	342,277	2915-57-3	bis(2-ethylhexyl) succinate	3
	C19H38N2O3	342,2882	4292-10-8	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	3
	C22H32O3	344,2351	434-05-9	Metenolone acetate	3
	C22H32O3	344,2351	520-85-4	Medroxyprogesteron	3
	C22H32O3	344,2351	2668-66-8	medrysone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C20H22O2Si2	350,1158		Degradation-Product	3
	C20H32O5	352,225	363-24-6	dinoprostone	3
	C20H32O5	352,225	35121-78-9	epoprostenol	3
	C21H39NO3	353,293	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3
	C20H26N4O2	354,2056	3811-75-4	Hexamidine	3
	C22H28NO3	354,2064	125-51-9	pipenzolate	3
	C16H34O6S	354,2076		2-(2-dodecyloxyethoxy)ethyl sulfonic acid	3
	C18H28O5S	356,1657	481-97-0	Estrone sulphate	3
	C21H40O4	356,2927	28510-23-8	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	3
	C21H40O4	356,2927	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	C21H42O4	358,3083	31566-31-1	stearic acid, monoester with glycerol	3
	C22H33NO3	359,246	139-62-8	cyclomethycaine	3
	C18H20FN3O4	362,1543		ofloxacin	1
	C15H21Cl2FN2O3	366,0913	81406-37-3	Fluroxypyr-meptyl	3
	C22H43NO3	369,3243	93-83-4	N,N-bis(2-hydroxyethyl)oleamide	3
	C22H42O4	370,3083	103-23-1	bis(2-ethylhexyl) adipate	3
	C22H42O4	370,3083	1330-86-5	diisooctyl adipate	3
	C22H28O5	372,1937	24916-90-3	9?,11?-epoxy-17,21-dihydroxy-16?-methylpregna-1,4-diene-3,20-dione	3
	C22H28O5	372,1937	599-33-7	prednylidene	3
	C22H30O5	374,2093	1172-63-0	Jasmolin II	3
	C22H30O5	374,2093	83-43-2	Methylprednisolone	3
	C17H20N2O6S	380,1042	61-32-5	Methicillin	3
	C23H24N4O2	388,1899		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	C24H38O4	390,277	117-84-0	Di-n-octylphthalate (DOP)	3
	C24H38O4	390,277	117-81-7	DEHP	3
	C24H38O4	390,277	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	C24H38O4	390,277	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	C23H38O5	394,2719	64318-79-2	gemeprost	3
	C18H26FN3O4S	399,1628		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	C20H34O8	402,2254	77-90-7	Tributylacetylcitrate	3
	C23H20N2O3S	404,1195	57-96-5	sulfinpyrazone	3
	C22H28F2O5	410,1905	2135-17-3	flumetasone	3
	C22H28F2O5	410,1905	2557-49-5	diflorasone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C25H48O4	412,3553	103-24-2	bis(2-ethylhexyl) azelate	3
	C24H30O6	414,2042	107724-20-9	eplerenone	3
	C24H30O6	414,2042		2,6-bis(4-ethylphenyl)perhydro-1,3,5,7-tetraoxanaphth-4-ylethane-1,2-diol	3
	C25H37NO4	415,2723	155206-00-1	Bimatoprost	3
	C25H37NO4	415,2723	89365-50-4	Salmeterol	3
	C26H42O4	418,3083	28553-12-0	Diisononyl phthalate (DINP)	3
	C25H42O5	422,3032	1448-36-8	methyl cholate	3
	C27H42O4	430,3083	472-11-7	ruscogenin	3
	C29H41NO4	467,3036	52485-79-7	Buprenorphin	3
	C30H37NO4	475,2723	126784-99-4	Ulipristal acetate	3
	C32H39NO4	501,2879	83799-24-0	fexofenadine	3
	C30H53N3O6	551,3934	173334-57-1	aliskiren	3
	C34H50O7	570,3557	5697-56-3	carbenoxolone	3
	C40H80NO8P	733,5622	63-89-8	Colfosceril-Palminat	3
	C48H69N3O6	783,5186	27676-62-6		3
Herring	C6H6FN	111,0484	371-40-4	4-fluoroaniline	3
	C2H2F3NO	113,0088	354-38-1	2,2,2-trifluoroacetamide	3
	C5H10O4	134,0579	4767-03-7	2,2-bis(hydroxymethyl)propionic acid	3
	C5H5N5	135,0545	73-24-5	adenine	3
	C5H12S2	136,038		2,2-Bis(methylthio)propane	3
	C6H7N3O	137,0589	54-85-3	isoniazid	3
	C7H5NO3	151,0269	552-89-6	2-nitrobenzaldehyde	3
	C7H6O4	154,0266	490-79-9	Gentisinsäure	3
	C7H6O4	154,0266	99-10-5	à-resorcylic acid	3
	C6H9N3O2	155,0695	4998-57-6	histidine	3
	C6H9N3O2	155,0695	36315-01-2	IN-J0290	3
	C6H9N3O2	155,0695	6642-31-5	6-amino-1,3-dimethyluracil	3
	C6H9N3O2	155,0695	6994-25-8	ethyl 3-amino-1H-pyrazole-4-carboxylate	3
	C10H10N2	158,0844	2243-62-1	1,5-naphthylenediamine	3
	C10H10N2	158,0844	479-27-6	1,8-naphthylenediamine	3
	C9H7NO2	161,0477	13031-41-9	4-cyanophenyl acetate	3
	C9H11NO2	166,0867		metolcarb	3
	C6H4N2O4	168,0171	528-29-0		3
	C6H9N3O3	171,0644	443-48-1	Metronidazole	3
	C6H6O4S	173,9987	98-67-9	4-hydroxybenzenesulfonic acid	3
	C13H11N	181,0891	1013-88-3	diphenylmethanimine	3
	C9H10O4	182,0579	94050-90-5	(R)-2-(4-hydroxyphenoxy)propanoic acid	3
	C12H12N2	184,1	92-87-5	benzidine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C12H12N2	184,1	101-54-2	N-(4-aminophenyl)aniline	3
	C12H17NO	192,1391		DEET	3
	C13H17NO	203,131	483-63-6	Crotamiton	3
	C13H17NO	203,131		3-(1-pyrrolidinyl)propiophenone	3
	C13H17NO	203,131	28178-42-9	2,6-diisopropylphenyl isocyanate	3
	C11H12N2O2	205,0978		4-hydroxyantipyrine	3
	C13H11N3	209,0953		Acridine-3,6-diamine	3
	C10H8ClN3O	221,0356	1698-60-8	chloridazon	3
	C12H15NO3	222,1127		carbofuran	3
	C4H6N4O3S2	222,995		acetazolamide	2
	C8H11NO5S	233,0358	68373-14-8	Sulbactam	3
	C12H14N2O3	234,1004	20857-92-5	1-(4-nitrobenzoyl)-piperidine	3
	C12H14N2O3	234,1004	65855-02-9	1-benzyl-5-ethoxyimidazolidine-2,4-dione	3
	C12H14N2O3	234,1004		4-(4,4-dimethyl-3-oxo-pyrazolidin-1-yl)-benzoic acid	3
	C12H16N2O3	237,124		carbetamide	3
	C15H19NO2	245,1416	53948-51-9	Bisnortilidin	3
	C16H21N3	255,1735	91-81-6	tripelennamine	3
	C17H19N3	265,1579	91-75-8	antazoline	3
	C17H19N3	265,1579	85650-52-8	mirtazapine	3
	C11H17N5O3	267,1331	30924-31-3	Cafaminol	3
	C20H21N	275,1674	303-53-7	cyclobenzaprine	3
	C21H21N	287,1674	129-03-3	cyproheptadine	3
	C21H21N	287,1674	65472-88-0	Naftifine	3
	C16H25N3O2	291,1947	67635-46-5	propionylprocainamide	3
	C21H25N	291,1987	5118-29-6	melitracene	3
	C21H25N	291,1987	91161-71-6	terbinafine	3
	C21H27N	293,2143	14334-40-8	pramiverin	3
	C21H27N	293,2143	15686-37-0	butriptyline	3
	C14H18N2O5	294,1216	81-14-1	Musk ketone	3
	C14H18N2O5	294,1216	22839-47-0	Aspartam	3
	C15H19N3O4	305,1376	114311-32-9	Imazamox	3
	C21H23NO	305,178	119356-77-3	dapoxetine	3
	C19H17NO3	307,1208	92-74-0	2'-ethoxy-3-hydroxy-2-naphthanilide	3
	C21H25NO	307,1936	86-13-5	Benztropine mesylate	3
	C21H30N2	310,2409		4,4'-methylenebis(2-isopropyl-6-methylaniline)	3
	C19H21NO3	311,1521	62-67-9	nalorphine	3
	C22H27NO	321,2093	524-83-4	ethybenztropine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C20H31N3O	329,2467		1-tetradecanoylbenzotriazole	3
	C23H25NO	331,1936	14089-87-3	1,1-diphenyl-1-methoxy-3-benzylaminopropane	3
	C17H25N3O2S	335,1667	121679-13-8	naratriptan	3
	C20H33NO3	335,246	468-61-1	oxeladin	3
	C19H23N3O3	341,1739	13424-56-1	nicotinoylprocaine	3
	C20H27N3O2	341,2103		UV stabilizers	3
	C20H29N3O2	343,226	85-79-0	dibucaine	3
	C16H19N3O4S	349,1096		metabolite BH 479-9 of Metazachlor	3
	C16H19N3O4S	349,1096	69-53-4	ampicillin	3
	C14H28NO3PS2	353,1248	24151-93-7	Piperophos	3
	C19H20N2O3S	356,1195	111025-46-8	Pioglitazone	3
	C20H20FNO4	357,1376	122008-85-9	Cyhalofop-butyl	3
	C22H27N3O2	365,2103	23465-76-1	caroverine	3
	C18H36N2O6	376,2573	57843-53-5	N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide	3
	C20H33N3O4	379,2471	56980-93-9	celiprolol	3
	C17H25N3O5S	383,1515	119478-56-7	meropenem	3
	C21H25N3O2S	383,1667	111974-69-7	quetiapine	3
	C22ClH41N2O2	400,2857	73833-37-1	2,2,4,4-tetramethyl-7-oxa-3,20-diazadispiro[5.1.11.2]henicosan-21-one hydrochloride	3
	C21H46NO4P	407,3164	58066-85-6	miltefosine	3
	C27H26N2O2	410,1994			3
	C27H42NO2	412,321		Benzethonium	3
	C26H26ClN3	415,1815	158876-82-5	Rupatadine	3
	C26H42N4O2	442,3308		N,N'-bis(2,2,6,6-tetramethyl-4-piperidyl)isophthalamide	3
	C24H29N3O4S	455,1879	84-97-9	Perazine	3
	C27H36O7	472,2461	86401-95-8	Methylprednisolonaceponat	3
	C24H46O7S	478,2964		1,4-diisodecyl-2-sulfosuccinic acid	3
	C22H48O12	504,3146	9051-49-4	Pentaerythritol, propoxylated	3
	C24H40N8O4	504,3173	58-32-2	dipyridamole	3
	C31H44O7	528,3087	51596-10-2	Milbemectin A3	3
	C35H36N2O3	532,2726		2'-anilino-6'-(N-ethyl-N-hexylamino)-3'-methylspiro(isobenzofuran-1(1H),9'-xanthen)-3-one	3
	C32H44O7	540,3087	126544-47-6	Ciclesonide	3
	C32H46O7	542,3244	51596-11-3	Milbemectin A4	3
	C34H50O7	570,3557	5697-56-3	carbenoxolone	3
	C41H76N2O15	836,5246	80214-83-1	roxithromycin	3
Cod Liver	C5 H8 O2	101,0598	80-62-6	Methyl methacrylate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C8 H11 N	122,0968	95-68-1	2,4-Dimethylaniline (2,4-Xylidine)	3
	C8 H9 N O	136,0766	103-84-4	Acetanilide	3
	C6 H12 N2 O3	161,093	1596-84-5	Daminozide	3
	C9 H11 N O2	166,0865	1129-41-5	Metolcarb	3
	C7 H11 N3 O2	170,0926	14885-29-1	Ipronidazole	3
	C6 H8 N2 O2 S	173,039	63-74-1	Sulfanilamide	3
	C10 H13 N O2	180,1015	122-42-9	IPC / Propham	3
	C12 H17 N O	192,1388	134-62-3	DEET / Diethyltoluamide	3
	C11 H12 N2 O2	205,0975	1672-63-5	4-Hydroxyantipyrine	3
	C12 H17 N O2	208,1338	3766-81-2	Fenobucarb (Baycarb)	3
	C10 H10 N4 O	225,0742	41394-05-2	Metamitron	3
	C14 H22 O	229,1556	33704-61-9	DPMI / Cashmeran	3
	C8 H8 N4 O3	231,0491	16004-43-6	2-NBA-SEM (2-NP-SCA)	3
	C8 H6 N4 O5	239,0421	67-20-9	Nitrofurantoin	3
	C12 H14 N2 S	241,0787	61676-87-7	Tifatol (Cymiazole)	3
	C8 H19 O2 P S2	243,0628	13194-48-4	Ethoprop (Ethoprophos)	3
	C6 H15 O2 P S3	247,0046	640-15-3	Thiometon	3
	C9 H12 N4 O3 S	257,0706	19077-97-5	N4-Acetylsulfaguanidin (Acetamide, N-(4-(((aminoiminomethyl)amino)sulfonyl)phenyl)-)	3
	C15 H15 N O3	258,1107	26171-23-3	Tolmetin	3
	C18 H26 O	259,2069	1506-02-1	AHTN / Tonalide (Fixolide)	3
	C8 H16 N O5 P	260,065	141-66-2	Dicrotophos (Bidrin)	3
	C11 H18 N4 O2	261,1328	23103-98-2	Pirimicarb	3
	C15 H21 N O4	280,1552	57837-19-1	Metalaxyl	3
	C13 H16 N4 O2	283,1166	5355-16-8	Diaveridin	3
	C19 H22 O2	283,1679	71109-09-6	Vedaprofen	3
	C19 H24 O2	285,1857	897-06-3	Boldione	3
	C20 H28 O	285,221	52-76-6	Lynestrenol	3
	C20 H32 O	289,2531	965-90-2	Ethylestrenol	3
	C12 H20 N4 O S	291,1259	57052-04-7	Isomethiozin	3
	C19 H30 O2	291,2327	521-18-6	Androstanolone	3
	C18 H22 O2	293,1499	80657-17-6	17-alpha-Trenbolon	3
	C19 H32 O2	293,2487	1852-53-5	17-beta-Dihydroandrosterone (3alpha Androstanediol)	3
	C18 H24 O2	295,1666	57-91-0	17alpha-Estradiol (alfatradiol)	3
	C14 H11 F3 N2 O2	297,0837	38677-85-9	Flunixin	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Oslofjord sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C18 H35 N O2	298,2737	118134-30-8	Spiroxamine	3
	C19 H39 N O	298,3107	24602-86-6	Tridemorph	3
	C20 H28 O2	301,2175	1231-93-2	Ethynodiol	3
	C20 H30 O2	303,2323	58-18-4	17-Methyltestosterone	3
	C20 H30 O2	303,2335	58-18-4	17-Methyltestosterone	3
	C19 H28 O3	305,2124	739-27-5	Ethiocolanolon (11-Ketoetiocholanolone)	3
	C20 H32 O2	305,2468	58-19-5	Drostanolone	3
	C15 H23 N3 O4	310,1761	33820-53-0	Isopropalin (Bifenthrin)	3
	C21 H30 O2	315,2315	57-83-0	Progesterone	3
	C16 H15 F2 N3 Si	316,1071	85509-19-9	Flusilazol	3
	C11 H12 N O4 P S2	318,0022	732-11-6	Phosmet (Imidan)	3
	C20 H32 O3	321,2431		Mutiline (8-alpha-hydroxy-Mutilin)	3
	C20 H28 O2	323,1986	1231-93-2	Ethynodiol	3
	C13 H16 N4 O6	325,1132	139-91-3	Furaltadone	3
	C21 H26 O3	327,197	34816-55-2	Moxestrol	3
	C22 H32 O2	329,2489	1239-79-8	16-alpha-Methylprogesteron	3
	C22 H26 O3	339,1946	28434-01-7	Bioresmethrin (Isatrin)	3
	C22 H28 O3	341,2106	51-98-9	Norethindrone acetate	3
	C12 H17 O4 P S2	343,0178	07.03.2597	Phenthoate (Fenthoate)	3
	C22 H30 O3	343,2272	3562-63-8	Megestrol	3
	C22 H32 O3	345,2425	520-85-4	Medroxyprogesterone	3
	C21 H30 O4	347,2223	50-22-6	Corticosterone	3
	C21 H28 O3	351,1935	121-21-1	Pyrethrin I	3
	C17 H19 F N4 O4	363,1464	115550-35-1	Marbofloxacin	3
	C21 H29 F O4	365,2109	337-03-1	Flugestone	3
	C23 H26 O3	373,1786	26002-80-2	Phenothrin	3
	C23 H32 O4	373,2371	56-47-3	Deoxycorticosterone acetate	3
	C24 H28 N3	381,2171	8004-87-3	Basic Violet 1 (Methyl Violet)	3
	C24 H32 O4	385,2365	113-38-2	Estradiol dipropionate	3
	C27 H33 N2	386,2716	18198-35-1	Brilliant Green (Ethyl Green)	3
	C24 H34 O4	387,2536	71-58-9	Medroxyprogesterone acetate	3
	C25 H38 O3	387,2894	15262-86-9	Testosterone isocapronate	3
	C20 H18 Cl N O6	426,0717	303-47-9	Ochratoxin A	3
	C32 H46 O7	543,331	51596-11-3	Milbemectin A4 (Milbemycin A4)	3
	C41 H79 N3 O12	806,5725	217500-96-4	Tulathromycin	3

Non-target screening results for LC-HR-QToF in negative ESI-mode analysis of the Oslofjord sample matrices					
Sample matrix	Molecular formula	RMM	CAS	Compound name	ID level
Krill	C8H2F17NO2S	497,9449	754-91-6	PFOSA	3
	C8HF17O3S	498,9288	1763-23-1	PFOS	3
Northern Shrimp	C8H2F17NO2S	497,9449	754-91-6	PFOSA	3
	C8HF17O3S	498,9288	1763-23-1	PFOS	3
	C10H4F17NO4S	555,9504	2991-50-6	PFOSAA	3
	C11HF21O2	562,9579	2058-94-8	PFUDA	3
	C10HF21O3S	598,926	335-77-3	PFDS	3
	C12HF23O2	612,9558	307-55-1	PFDoA	3
	C13HF25O2	662,9469	72629-94-8	PFTrDA	3
Herring	C8H2F17NO2S	497,9449	754-91-6	PFOSA	3
	C8HF17O3S	498,9288	1763-23-1	PFOS	3
Cod liver	C8H2F17NO2S	497,9449	754-91-6	PFOSA	3
	C8HF17O3S	498,9288	1763-23-1	PFOS	3

Non-target screening results for GCxGC-LRToF analysis of the Mjøsa sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
Zooplankton	C6Cl6	288	93952-14-8	Hexachlorobenzene	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H9Cl5	364	104215-84-1	p,p'-DDT	1
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
Mysis	C16H16O	224	954-16-5	Benzophenone, 2,4,6-trimethyl-	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H9Cl5	364	104215-84-1	p,p'-DDT	1
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
Small Smelt	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
Large Smelt	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1

Non-target screening results for GCxGC-LRToF analysis of the Mjøsa sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level
	C14H10Cl4	318	72-54-8	p,p-DDD	1
	C18H15O4P	326	115-86-6	Triphenyl phosphate	1
	C14H9Cl5	352	50-29-3	p,p'-DDT	1
	C14H9Cl5	352	53-19-0	o,p'-DDD	2
	C12H4Cl6	358	185376-58-3	Hexachlorobiphenyl	1
	C10H5Cl9	440	39765-80-5	trans-Nonachlor	2
	C10H5Cl9	440	5103-73-1	cis-Nonachlor	2
Vendace	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H10Cl4	320	53-19-0	o,p'-DDD	2
	C14H9Cl5	352	104215-84-1	p,p'-DDT	1
	C14H9Cl5	352	789-02-6	o,p'-DDT	3
	C12H4Cl6	358	35694-06-5	Hexachlorobiphenyl	1
	C12H4Cl6	370	185376-58-3	Hexachlorobiphenyl	1
Trout	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C6H12Cl3O4P	284	115-96-8	Tri(2-chloroethyl) phosphate	1
	C14H8Cl4	316	72-55-9	p,p'-DDE	1
	C14H10Cl4	318	72-54-8	p,p'-DDD	1
	C14H10Cl4	318	4329-12-8	m,p'-DDD	3
	C18H15O4P	326	115-86-6	Triphenyl phosphate	1
	C14H9Cl5	352	104215-84-1	p,p'-DDT	1
	C14H9Cl5	352	789-02-6	o,p-DDT	2
	C12H4Cl6	358	74472-41-6	Hexachlorobiphenyl	1
	C12H4Cl6	358	35065-28-2	Hexachlorobiphenyl	1
	C10H5Cl7	370	76-44-8	Heptachlor	3
	C10H6Cl8	406	5103-71-9	cis-chlordane	2
	C10H5Cl9	440	39765-80-5	trans/cis-Nonachlor	2
	C10H5Cl9	440	5103-73-1	Trans/cis-Nonachlor	2

Non-target screening results for GC-HRToF analysis of the Mjøsa sample matrices					
Matrix	Molecular formula	RMM	CAS	Compound name	ID level

Mysis	C13H10O	182.0732	119-61-9	Benzophenone	1
	C18H26O	258.1984	1222-05-5	Galaxolide	1
	C12H14O4	222.0892	84-66-2	Diethyl phthalate	2
	C20H36O2	308.2715	554-35-4	Linoleic acid ethyl ester	3
	C21H40O2	324.3028	22147-34-8	Elaidic acid propyl ester	3
	C20H34O8	402.2254	77-90-7	Tributyl acetylcitrate	3
Zooplankton	C12H14O4	222.0892	84-66-2	Diethyl phthalate	2
	C21H40O2	324.3028	22147-34-8	Elaidic acid, isopropyl ester	2
	C18H36O	268.2766		Methyl n-hexadecyl ketone	3
Vendace	C18H26O	258.1984	1222-05-5	Galaxolide	1
	C12H14O4	222.0892	84-66-2	Diethyl phthalate	2
	C14H18Cl4	315.938		DDE	2
	C18H15O4P	326.0708	115-86-6	Triphenyl phosphate	2
	C9H10O	134.0732		Phenyl propanone	3
	C19H20O4	312.1362		Benzyl butyl phthalate	3
Smelt	C18H26O	258.1984	1222-05-5	Galaxolide	1
	C12H14O4	222.0892	84-66-2	Diethyl phthalate	2
	C19H38O2	298.2872	143-91-6	Isopropyl palmitate	2
	C21H42O2	326.3185	112-10-7	Isopropyl stearate	2
	C24H38O4	390.2770	117-81-7	Bis(2-ethylhexyl) phthalate	2
	C20H14O2S	318.0714	32390-26-4	Binaphthyl sulfone	3
Brown Trout	C13H10O	182.0732	119-61-9	Benzophenone	1
	C12H14O4	222.0892	84-66-2	Diethyl phthalate	2
	C16H24O	232.1827	10541-56-7	p-Octylacetophenone	2
	C17H34O2	270.2559	110-27-0	Isopropyl myristate	2
	C16H22O4	278.1518	84-74-2	Dibutyl phthalate	2
	C14H18Cl4	315.938		DDE	2
	C18H18Cl2O	320.0735		3-Butanone, 1,1-bis(4-chlorophenyl)-2,2-dimethyl-	2
	C12H5Cl5	323.8834		Pentachlorobiphenyl	2
	C12H5Cl5	323.8834		Pentachlorobiphenyl	2
	C12H4Cl6	357.8444		hexachlorobiphenyl	2
	C12H4Cl6	357.8444		hexachlorobiphenyl	2
	C12H4Cl6	357.8444		hexachlorobiphenyl	2

	C12H3Cl7	391.8054		heptachlorobiphenyl	2
	C12H3Cl7	391.8054		heptachlorobiphenyl	2
	C14H14N2	210.1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210.1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210.1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C14H14N2	210.1157	57964-39-3	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	3
	C18H36	252.2817		Octadecene	3
	C12H27O4P	266.1645	126-73-8	Tributyl phosphate	3
	C20H38	278.2974		3,7,11,15-Tetramethyl-2-hexadecen-1-ol	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
Mysis	71,0735	C4H9N	123-75-1	pyrrolidine	3
	89,0477	C3H7NO2	625-51-4	N-(hydroxymethyl)acetamide	3
	89,0477	C3H7NO2	107-95-9	ß-alanine	3
	89,0477	C3H7NO2	107-97-1	sarcosine	3
	89,0477	C3H7NO2	56-41-7	L-alanine	3
	93,0578	C6H7N	62-53-3	Aniline	3
	93,0578	C6H7N	108-99-6	3-methylpyridine	3
	102,0681	C5H10O2	75-98-9	pivalic acid	3
	102,0681	C5H10O2	108-21-4	isopropyl acetate	3
	102,0681	C5H10O2	109-52-4	valeric acid	3
	102,0681	C5H10O2	109-60-4	propyl acetate	3
	102,0681	C5H10O2	505-65-7	1,3-dioxepane	3
	102,0681	C5H10O2	97-99-4	tetrahydrofurfuryl alcohol	3
	102,0681	C5H10O2	116-53-0	2-methylbutyric acid	3
	102,0681	C5H10O2	503-74-2	isovaleric acid	3
	115,0633	C5H9NO2	4394-85-8	N-Formylmorpholine	3
	115,0633	C5H9NO2	147-85-3	L-proline	3
	115,0633	C5H9NO2	923-02-4	N-(hydroxymethyl)methacrylamide	3
	115,0633	C5H9NO2	14205-39-1	methyl 3-aminocrotonate	3
	120,0575	C8H8O	96-09-3	(epoxyethyl)benzene	3
	120,0575	C8H8O	98-86-2	acetophenone	3
	120,0939	C9H12	98-82-8	Isopropylbenzol	3
	120,0939	C9H12	95-63-6	1,2,4-trimethylbenzene	3
	120,0939	C9H12	108-67-8	mesitylene	3
	120,0939	C9H12	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3
	120,0939	C9H12	3048-64-4	5-vinylnorborn-2-ene	3
	125,0147	C2H7NO3S	107-35-7	taurine	3
	132,0939	C10H12	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3
	132,0939	C10H12	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	132,0939	C10H12	768-56-9	4-phenylbut-1-ene	3
	134,0732	C9H10O	93-55-0	propiophenone	3
	134,0732	C9H10O	104-54-1	cinnamyl alcohol	3
	134,1096	C10H14	99-87-6	p-cymene	3
	134,1096	C10H14	4488-57-7	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	3
	134,1096	C10H14	25340-17-4	diethylbenzene	3
	134,1096	C10H14	68411-44-9	Benzene, butyl-, branched and linear	3
	134,1096	C10H14	105-05-5	1,4-diethylbenzene	3
	135,0545	C5H5N5	73-24-5	adenine	3
	143,0946	C7H13NO2	7747-35-5	7a-ethyldihydro-1H,3H,5H-	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
				oxazolo[3,4-c]oxazole	
	143,0946	C7H13NO2	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	143,9743	C2H6ClO3P	16672-87-0	Ethephon	3
	147,0718	C6H13NOS	141-98-0	O-isopropyl ethylthiocarbamate	3
	148,016	C8H4O3	85-44-9	phthalic anhydride	3
	148,0524	C9H8O2	621-82-9	cinnamic acid	3
	152,0334	C5H4N4O2	69-89-6	xanthine	3
	152,0334	C5H4N4O2	2465-59-0	oxypurinol	3
	152,095	C8H12N2O	2814-20-2	G27550	3
	154,0611	C6H7N3O2	86490-48-4	nitrophenylhydrazine	3
	158,0844	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	158,0844	C10H10N2	479-27-6	1,8-naphthylenediamine	3
	158,1096	C12H14	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	158,1096	C12H14	3748-13-8	m-bis(1-methylvinyl)benzene	3
	161,1052	C7H15NO3	541-15-1	Levocarnitin	3
	161,1056	C6H19NSi2	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	162,0317	C9H6O3	93-35-6	7-hydroxycoumarine	3
	162,1409	C12H18	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	162,1409	C12H18	7397-06-0		3
	162,1409	C12H18	4904-61-4	cyclododeca-1,5,9-triene	3
	162,1409	C12H18	99-62-7	1,3-diisopropylbenzene	3
	162,1409	C12H18	100-18-5	1,4-diisopropylbenzene	3
	162,1409	C12H18	25321-09-9	diisopropylbenzene	3
	164,0473	C9H8O3	156-06-9	phenylpyruvic acid	3
	164,0473	C9H8O3	15206-55-0	methyl benzoylformate	3
	164,1201	C11H16O	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	164,1201	C11H16O	88-60-8	6-tert-butyl-m-cresol	3
	164,1201	C11H16O	2409-55-4	2-tert-butyl-p-cresol	3
	164,1201	C11H16O	583-03-9	fenipentol	3
	165,079	C9H11NO2	94-09-7	benzocaine	3
	165,079	C9H11NO2	51-66-1	methacetin	3
	165,079	C9H11NO2	1129-41-5	Metolcarb	3
	165,079	C9H11NO2	938-73-8	Ethenzamide	3
	165,079	C9H11NO2	18595-18-1	Benzoic acid, 3-amino-4-methyl-, methyl ester	3
	165,079	C9H11NO2	24461-61-8	methyl (R)-aminophenylacetate	3
	166,063	C9H10O3	120-47-8	ethyl 4-hydroxybenzoate	3
	166,063	C9H10O3	121-32-4	ethyl vanillin	3
	166,063	C9H10O3	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	166,063	C9H10O3	11070-44-3	tetrahydromethylphthalic anhydride	3
	166,063	C9H10O3	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	166,0841	C6H14O5	59113-36-9	oxybispropanediol	3
	170,0943	C9H14O3	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	170,0943	C9H14O3	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	180,0423	C9H8O4	50-78-2	acetylsalicyl acid	3
	182,0732	C13H10O	119-61-9	benzophenone	3
	182,0732	C13H10O	3218-36-8	p-phenylbenzaldehyde	3
	188,1565	C14H20	81-03-8		3
	188,1565	C14H20	1203-17-4	1,1,2,3,3-pentamethylindan	3
	193,1103	C11H15NO2	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	193,1103	C11H15NO2	94-25-7	butamben	3
	193,1103	C11H15NO2	42542-10-9	3,4-methylenedioxymethamphetamine	3
	193,1103	C11H15NO2	1795-96-6	phenylalanine, ethyl ester	3
	193,1103	C11H15NO2	7298-73-9	N-Methylphenacetine	3
	193,1103	C11H15NO2	2631-40-5	Isoprocarb	3
	193,1103	C11H15NO2	2686-99-9	3,4,5-Trimethacarb	3
	193,1103	C11H15NO2	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	193,1103	C11H15NO2	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	194,0943	C11H14O3	94-26-8	Butyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	614-45-9	tert-butyl perbenzoate	3
	198,162	C12H22O2	88-41-5		3
	198,162	C12H22O2	111-81-9	methyl undec-10-enoate	3
	198,162	C12H22O2	688-84-6	2-ethylhexyl methacrylate	3
	198,162	C12H22O2	51000-52-3	vinyl neodecanoate	3
	198,162	C12H22O2		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	198,162	C12H22O2	89-48-5	menthyl acetate	3
	198,162	C12H22O2	150-84-5	citronellyl acetate	3
	198,162	C12H22O2	713-95-1	dodecan-5-olide	3
	198,162	C12H22O2	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	198,162	C12H22O2	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	203,1162	C8H21NOSi2	10416-59-8	trimethylsilyl N-trimethylsilylacetamidate	3
	204,115	C13H16O2	947-19-3	Methanone, Irgacure 184	3
	204,115	C13H16O2	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	204,115	C13H16O2	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	204,1514	C14H20O	80-54-6	Bucinal	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	204,1514	C14H20O	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	206,1307	C13H18O2	15687-27-1	Ibuprofen	3
	206,1307	C13H18O2	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	210,1021	C8H19O4P		Di-tert-butyl hydrogen phosphate	3
	210,1984	C14H26O		Degradation-Product	3
	210,1984	C14H26O	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	212,1161	C10H16N2O3	125-40-6	secbutabarbital	3
	212,1161	C10H16N2O3	77-28-1	butobarbital	3
	218,2035	C16H26	68648-87-3		3
	220,1463	C14H20O2	719-22-2	2,6-Di-tert-butylquinone	3
	227,1885	C13H25NO2		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	234,1256	C14H18O3	49763-96-4	stiripentol	3
	234,162	C15H22O2	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	234,162	C15H22O2	5444-75-7	2-ethylhexyl benzoate	3
	234,1984	C16H26O	54464-57-2	OTNE	3
	234,1984	C16H26O	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O		Degradation-Product	3
	234,1984	C16H26O	68155-66-8		3
	234,1984	C16H26O	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	234,1984	C16H26O	121158-58-5	Phenol, dodecyl-, branched	3
	236,1776	C15H24O2	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	240,1514	C17H20O	15087-24-8	3-benzylidenecamphor	3
	241,277	C16H35N	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	241,277	C16H35N	112-75-4	dimethyl(tetradecyl)amine	3
	241,277	C16H35N	1120-48-5	dioctylamine	3
	242,0903	C10H14N2O5	3424-98-4	Telbivudine	3
	242,0903	C10H14N2O5	50-89-5	thymidine	3
	242,2035	C18H26	1087-02-1	p-Dicyclohexylbenzene	3
	243,0855	C9H13N3O5	147-94-4	cytarabine	3
	244,1787	C12H24N2O3	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	246,162	C16H22O2		Degradation-Product	3
	246,2348	C18H30	2719-62-2	6-Phenyldodecane	3
	246,2348	C18H30	25265-78-5	tetrapropylenebenzene	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	248,1042	C6H20N2O6S	5080-22-8	N-isopropylhydroxylamine	3
	248,1049	C14H16O4	5292-53-5	diethyl (phenylmethylene)malonate	3
	248,1776	C16H24O2	18017-73-7	10-Phenyldecanoic acid	3
	248,1776	C16H24O2	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	250,1933	C16H26O2		Degradation-Product	3
	250,1933	C16H26O2	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	250,1933	C16H26O2	79-74-3	2,5-di-tert-pentylhydroquinone	3
	252,2089	C16H28O2	30507-70-1	(Z,E)-tetradeca-9,12-dienyl acetate	3
	253,2406	C16H31NO	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	253,2406	C16H31NO	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	254,2246	C16H30O2	142-90-5	dodecyl methacrylate	3
	258,1984	C18H26O	1222-05-5	Galaxolide	3
	258,1984	C18H26O		1-(4-(trans-4-butylcyclohexyl)phenyl)ethanone	3
	260,0507	C14H12O3S	33005-95-7	tiaprofenic acid	3
	262,2297	C18H30O	5892-47-7	2,4,6-tri-sec-butylphenol	3
	265,1678	C15H23NO3	6452-71-7	oxprenolol	3
	266,1307	C18H18O2	13029-44-2	Dienestrol	3
	266,1307	C18H18O2	517-09-9	Equilenin	3
	266,1307	C18H18O2	63250-25-9	isopropyldibenzoylmethane	3
	266,1552	C12H26O4S		dodecyl sulfuric acid	3
	266,1552	C12H26O4S		2-butyloctyl-sulfonic acid	3
	266,1647	C12H27O4P	126-73-8	tributyl phosphate	3
	266,1647	C12H27O4P	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	266,1882	C16H26O3	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	266,1882	C16H26O3	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	266,261	C18H34O		Degradation-Product	3
	267,0968	C10H13N5O4	58-61-7	adenosine	3
	267,0968	C10H13N5O4	30516-87-1	Zidovudine	3
	268,2402	C17H32O2	21643-42-5	tetradecyl acrylate	3
	269,3083	C18H39N	112-69-6	hexadecyldimethylamine	3
	269,3083	C18H39N	124-30-1	octadecylamine	3
	272,0789	C9H13ClN6O2	42471-28-3	nimustine	3
	272,1776	C18H24O2	50-28-2	17-beta-Estradiol	3
	272,1776	C18H24O2	57-91-0	alfatradiol	3
	274,1933	C18H26O2	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	274,1933	C18H26O2	434-22-0	nandrolone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	276,1725	C17H24O3	456-59-7	cyclandelate	3
	276,1725	C17H24O3	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	276,2121	C14H32O3Si	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	3
	276,2121	C14H32O3Si	2943-75-1	triethoxyoctylsilane	3
	277,1699	C19H21N2	524-81-2	mebhydroline	3
	278,1518	C16H22O4	84-74-2	Dibutyl phthalate	3
	278,1518	C16H22O4	84-69-5	diisobutyl phthalate	3
	278,1518	C16H22O4	1962-75-0	dibutyl terephthalate	3
	278,2246	C18H30O2		Di-nonylpheno	3
	278,2246	C18H30O2		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	278,2246	C18H30O2	506-26-3	gamolenic acid	3
	280,2402	C18H32O2	60-33-3	linoleic acid	3
	281,2719	C18H35NO	1593-77-7	Dodemorph	3
	282,2559	C18H34O2	112-80-1	Oleic acid	3
	282,2559	C18H34O2	2549-53-3	tetradecyl methacrylate	3
	283,2875	C18H37NO	124-26-5	stearamide	3
	284,214	C20H28O	52-76-6	lynestrenol	3
	284,2351	C17H32O3		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	286,1933	C19H26O2	63-05-8	Androstendion	3
	286,1933	C19H26O2	846-48-0	boldenone	3
	286,2144	C16H30O4	6846-50-0	TXIB	3
	286,2144	C16H30O4	7491-02-3	diisopropyl sebacate	3
	286,2297	C20H30O	68-26-8	retinol	3
	288,2089	C19H28O2	481-30-1	Epitestosterone	3
	288,2089	C19H28O2	58-22-0	Testosterone	3
	288,2089	C19H28O2	53-43-0	prasterone	3
	288,2089	C19H28O2	1091-93-6	3-methoxyestra-2,5(10)-dien-17?-ol	3
	290,1882	C18H26O3	5466-77-3	Ethylhexyl methoxycinnamate	3
	290,2246	C19H30O2	521-18-6	androstanolone	3
	292,2038	C18H28O3	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	292,2766	C20H36O	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	294,2195	C18H30O3	2315-61-9	4-Octylphenol di-ethoxylate	3
	294,2216	C21H28N	57982-78-2	budipine	3
	297,2668	C18H35NO2	118134-30-8	Spiroxamine	3
	298,1933	C20H26O2	68-22-4	Norethisteron	3
	298,2508	C18H34O3	13040-19-2	diricinoleate	3
	299,1521	C18H21NO3	125-29-1	Hydrocodone	3
	299,1521	C18H21NO3	76-57-3	codeine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	299,1521	C18H21NO3	968-46-7	deanol benzilate	3
	300,2089	C20H28O2	5300-03-8	Alitretinoin	3
	300,2089	C20H28O2	1740-19-8	Abieta-8,11,13-trien-18-oic acid	3
	300,2089	C20H28O2	4759-48-2	Isotretinoin	3
	300,2089	C20H28O2	57144-06-6	3-methoxyandrosta-3,5-dien-17-one	3
	300,2664	C18H36O3	106-14-9	12-hydroxystearic acid	3
	301,2406	C20H31NO	144-11-6	trihexyphenidyl	3
	302,2246	C20H30O2	58-18-4	17-alpha-Methyltestosterone	3
	302,2246	C20H30O2	153-00-4	metenolone	3
	304,2402	C20H32O2	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	304,2402	C20H32O2	1424-00-6	mesterolone	3
	309,2668	C19H35NO2	77-19-0	dicyclomine	3
	310,2297	C22H30O	54024-22-5	Desogestrel	3
	310,2508	C19H34O3	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	312,195	C18H24N4O	109889-09-0	granisetron	3
	314,155	C19H23ClN2	303-49-1	clomipramine	3
	314,2246	C21H30O2	13956-29-1	cannabidiol	3
	314,2246	C21H30O2	1972-08-3	delta(9)-tetrahydrocannabinol	3
	314,2246	C21H30O2	57-83-0	Progesteron	3
	314,2246	C21H30O2	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	314,2457	C18H34O4	109-43-3	dibutyl sebacate	3
	314,2457	C18H34O4	110-33-8	dihexyl adipate	3
	314,2457	C18H34O4	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	314,2457	C18H34O4	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	314,2457	C18H34O4	871-70-5	1,18-octadecanedioic acid	3
	316,2038	C20H28O3	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	316,2038	C20H28O3	2137-18-0	gestonorone	3
	320,2351	C20H32O3		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3
	320,2385	C17H36O3S	111360-16-8	2-hexyldecyl mesylate	3
	322,2144	C19H30O4	106807-78-7	2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C)	3
	327,3137	C20H41NO2	111-57-9	N-(2-hydroxyethyl)stearamide	3
	328,2402	C22H32O2	127-47-9	retinyl acetate	3
	328,2614	C19H36O4	56519-71-2	propane-1,3-diyl dioctanoate	3
	330,1831	C20H26O4	84-61-7	dicyclohexyl phthalate	3
	330,3287	C24H42	4445-07-2	octadecylbenzene	3
	333,1608	C18H24ClN3O	119168-77-3	Tebufenpyrad	3
	333,1608	C18H24ClN3O	125225-28-7	Ipconazole	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	334,1441	C16FH19N4O3	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	335,1764	C18H26ClN3O	118-42-3	Hydroxychloroquine	3
	336,2512	C17H36O6	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	337,3345	C22H43NO		docos-13-enamide, Amides, C22 (unsaturated)	3
	338,2457	C20H34O4	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	342,1852	C24H23NO	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	342,2195	C22H30O3	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	342,2195	C22H30O3	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	342,2559	C23H34O2	7069-42-3	retinyl propionate	3
	342,277	C20H38O4	762-12-9	bisdecanoyl peroxide	3
	342,277	C20H38O4	2915-57-3	bis(2-ethylhexyl) succinate	3
	344,2351	C22H32O3	434-05-9	Metenolone acetate	3
	344,2351	C22H32O3	520-85-4	Medroxyprogesteron	3
	344,2351	C22H32O3	2668-66-8	medrysone	3
	352,225	C20H32O5	363-24-6	dinoprostone	3
	352,225	C20H32O5	35121-78-9	epoprostenol	3
	353,293	C21H39NO3	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3
	354,3134	C22H42O3		(3S,4S)-3-hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone	3
	356,1657	C18H28O5S	481-97-0	Estrone sulphate	3
	358,3083	C21H42O4	31566-31-1	stearic acid, monoester with glycerol	3
	360,2301	C22H32O4	8003-24-5	4-methoxy-3-tert-butylphenol	3
	360,2301	C22H32O4	78919-13-8	Iloprost	3
	366,0913	C15H21Cl2FN2O3	81406-37-3	Fluroxypyr-meptyl	3
	366,2195	C24H30O3	67392-87-4	drospirenone	3
	370,3083	C22H42O4	103-23-1	bis(2-ethylhexyl) adipate	3
	370,3083	C22H42O4	1330-86-5	diisooctyl adipate	3
	388,1899	C23H24N4O2		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	390,277	C24H38O4	117-84-0	Di-n-octylphthalate (DOP)	3
	390,277	C24H38O4	117-81-7	DEHP	3
	390,277	C24H38O4	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	390,277	C24H38O4	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	392,2927	C24H40O4	474-25-9	chenodeoxycholic acid	3
	392,2927	C24H40O4	128-13-2	ursodeoxycholic acid	3
	394,2719	C23H38O5	64318-79-2	gemeprost	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	398,2433	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	3
	400,3341	C27H44O2	41294-56-8	alphacalcidol	3
	402,2254	C20H34O8	77-90-7	Tributylacetylcitrate	3
	404,1195	C23H20N2O3S	57-96-5	sulfinpyrazone	3
	410,1905	C22H28F2O5	2135-17-3	flumetasone	3
	410,1905	C22H28F2O5	2557-49-5	diflorasone	3
	412,3553	C25H48O4	103-24-2	bis(2-ethylhexyl) azelate	3
	415,2723	C25H37NO4	155206-00-1	Bimatoprost	3
	415,2723	C25H37NO4	89365-50-4	Salmeterol	3
	418,3083	C26H42O4	28553-12-0	Diisononyl phthalate (DINP)	3
	422,3032	C25H42O5	1448-36-8	methyl cholate	3
	430,3083	C27H42O4	472-11-7	ruscogenin	3
	440,2345	C22H36N2O5S	144494-65-5	tirofiban	3
	467,3036	C29H41NO4	52485-79-7	Buprenorphin	3
	475,2723	C30H37NO4	126784-99-4	Ulipristal acetate	3
	501,2879	C32H39NO4	83799-24-0	fexofenadine	3
	515,2917	C26H45NO7S	81-24-3	taurocholic acid	3
	733,5622	C40H80NO8P	63-89-8	Colfosceril-Palminat	3
Small Smelt	102,1277	C6H16N	927-62-8	N,N-dimethylbutylamine	3
	111,0484	C6H6FN	371-40-4	4-fluoroaniline	3
	113,0088	C2H2F3NO	354-38-1	2,2,2-trifluoroacetamide	3
	116,1303	C6H16N2	694-83-7	cyclohex-1,2-ylenediamine	3
	130,0994	C7H14O2	111-14-8	heptanoic acid	3
	130,0994	C7H14O2	123-92-2	isopentyl acetate	3
	130,0994	C7H14O2		2-(alkoxyalkyl)oxolane	3
	130,0994	C7H14O2	106-70-7	methyl hexanoate	3
	130,0994	C7H14O2	7452-79-1	ethyl 2-methylbutyrate	3
	134,0579	C5H10O4	4767-03-7	2,2-bis(hydroxymethyl)propionic acid	3
	134,0943	C6H14O3	111-96-6	Diglyme (Diethylenglycol dimethyl ether)	3
	134,0943	C6H14O3	77-99-6	propylidynetrimethanol	3
	134,0943	C6H14O3	111-90-0	2-(2-ethoxyethoxy)ethanol	3
	134,0943	C6H14O3	25265-71-8	oxydipropanol	3
	134,0943	C6H14O3	25322-69-4	Propane-1,2-diol, propoxylated	3
	135,0545	C5H5N5	73-24-5	adenine	3
	136,038	C5H12S2		2,2-Bis(methylthio)propane	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	137,0589	C6H7N3O	54-85-3	isoniazid	3
	151,0269	C7H5NO3	552-89-6	2-nitrobenzaldehyde	3
	154,0266	C7H6O4	490-79-9	Gentisinsäure	3
	154,0266	C7H6O4	99-10-5	à-resorcylic acid	3
	155,0695	C6H9N3O2	4998-57-6	histidine	3
	155,0695	C6H9N3O2	36315-01-2	IN-J0290	3
	155,0695	C6H9N3O2	6642-31-5	6-amino-1,3-dimethyluracil	3
	155,0695	C6H9N3O2	6994-25-8	ethyl 3-amino-1H-pyrazole-4-carboxylate	3
	158,0844	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	158,0844	C10H10N2	479-27-6	1,8-naphthylenediamine	3
	161,0477	C9H7NO2	13031-41-9	4-cyanophenyl acetate	3
	168,0171	C6H4N2O4	528-29-0		3
	171,0644	C6H9N3O3	443-48-1	Metronidazole	3
	173,9987	C6H6O4S	98-67-9	4-hydroxybenzenesulfonic acid	3
	181,0891	C13H11N	1013-88-3	diphenylmethanimine	3
	182,0579	C9H10O4	94050-90-5	(R)-2-(4-hydroxyphenoxy)propanoic acid	3
	184,1	C12H12N2	92-87-5	benzidine	3
	184,1	C12H12N2	101-54-2	N-(4-aminophenyl)aniline	3
	186,0856	C10H12F2O		1-butoxy-2,3-difluorobenzene	3
	203,131	C13H17NO	483-63-6	Crotamiton	3
	203,131	C13H17NO		3-(1-pyrrolidinyl)propiophenone	3
	203,131	C13H17NO	28178-42-9	2,6-diisopropylphenyl isocyanate	3
	209,0953	C13H11N3		Acridine-3,6-diamine	3
	221,0356	C10H8ClN3O	1698-60-8	chloridazon	3
	221,0841	C15H11NO	92-71-7	2,5-diphenyloxazole	3
	233,0358	C8H11NO5S	68373-14-8	Sulbactam	3
	234,1004	C12H14N2O3	20857-92-5	1-(4-nitrobenzoyl)-piperidine	3
	234,1004	C12H14N2O3	65855-02-9	1-benzyl-5-ethoxyimidazolidine-2,4-dione	3
	234,1004	C12H14N2O3		4-(4,4-dimethyl-3-oxo-pyrazolidin-1-yl)-benzoic acid	3
	245,1416	C15H19NO2	53948-51-9	Bisnortilidin	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	255,1735	C16H21N3	91-81-6	tripelennamine	3
	265,1579	C17H19N3	91-75-8	antazoline	3
	265,1579	C17H19N3	85650-52-8	mirtazapine	3
	267,1331	C11H17N5O3	30924-31-3	Cafaminol	3
	275,1674	C20H21N	303-53-7	cyclobenzaprine	3
	287,1674	C21H21N	65472-88-0	Naftifine	3
	291,1987	C21H25N	5118-29-6	melitracene	3
	291,1987	C21H25N	91161-71-6	terbinafine	3
	294,1216	C14H18N2O5	81-14-1	Musk ketone	3
	294,1216	C14H18N2O5	22839-47-0	Aspartam	3
	305,1376	C15H19N3O4	114311-32-9	Imazamox	3
	305,178	C21H23NO	119356-77-3	dapoxetine	3
	307,1208	C19H17NO3	92-74-0	2'-ethoxy-3-hydroxy-2-naphthanilide	3
	310,2409	C21H30N2		4,4'-methylenebis(2-isopropyl-6-methylaniline)	3
	311,1521	C19H21NO3	62-67-9	nalorphine	3
	315,1987	C23H25N	13042-18-7	fendiline	3
	321,2093	C22H27NO	524-83-4	ethybenztropine	3
	329,2467	C20H31N3O		1-tetradecanoylbenzotriazole	3
	331,1936	C23H25NO	14089-87-3	1,1-diphenyl-1-methoxy-3-benzylaminopropane	3
	335,1667	C17H25N3O2S	121679-13-8	naratriptan	3
	335,246	C20H33NO3	468-61-1	oxeladin	3
	341,1739	C19H23N3O3	13424-56-1	nicotinoylprocaine	3
	341,2103	C20H27N3O2		UV stabilizers	3
	343,226	C20H29N3O2	85-79-0	dibucaine	3
	349,1096	C16H19N3O4S		metabolite BH 479-9 of Metazachlor	3
	349,1096	C16H19N3O4S	69-53-4	ampicillin	3
	351,2311	C22H29N3O	25973-55-1	2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol	3
	356,1195	C19H20N2O3S	111025-46-8	Pioglitazone	3
	357,1376	C20H20FNO4	122008-85-9	Cyhalofop-butyl	3
	364,321	C23H42NO2	19379-90-9	Benzoxonium	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	365,2103	C22H27N3O2	23465-76-1	caroverine	3
	379,226	C23H29N3O2	153-87-7	Oxypertine	3
	379,2471	C20H33N3O4	56980-93-9	celiprolol	3
	383,1515	C17H25N3O5S	119478-56-7	meropenem	3
	383,1667	C21H25N3O2S	111974-69-7	quetiapine	3
	387,2522	C22H33N3O3	4388-82-3	barbexaclone	3
	400,2857	C22ClH41N2O2	73833-37-1	2,2,4,4-tetramethyl-7-oxa-3,20-diazadispiro[5.1.11.2]henicosan-21-one hydrochloride	3
	407,3164	C21H46NO4P	58066-85-6	miltefosine	3
	415,1815	C26H26ClN3	158876-82-5	Rupatadine	3
	455,1879	C24H29N3O4S	84-97-9	Perazine	3
	472,2461	C27H36O7	86401-95-8	Methylprednisolonaceponat	3
	504,3146	C22H48O12	9051-49-4	Pentaerythritol, propoxylated	3
	504,3173	C24H40N8O4	58-32-2	dipyridamole	3
	528,3087	C31H44O7	51596-10-2	Milbemectin A3	3
	532,2726	C35H36N2O3		2'-anilino-6'-(N-ethyl-N-hexylamino)-3'-methylspiro(isobenzofuran-1(1H),9'-xanthen)-3-one	3
	540,3087	C32H44O7	126544-47-6	Ciclesonide	3
	570,3557	C34H50O7	5697-56-3	carbenoxolone	3
	655,768	C19H16Br4O6		Degradation-Product	3
	836,5246	C41H76N2O15	80214-83-1	roxithromycin	3
Smelt	89,0477	C3H7NO2	625-51-4	N-(hydroxymethyl)acetamide	3
	89,0477	C3H7NO2	79-46-9	2-nitropropane	3
	89,0477	C3H7NO2	107-95-9	ß-alanine	3
	89,0477	C3H7NO2	107-97-1	sarcosine	3
	89,0477	C3H7NO2	56-41-7	L-alanine	3
	93,0578	C6H7N	62-53-3	Aniline	3
	93,0578	C6H7N	108-99-6	3-methylpyridine	3
	102,0681	C5H10O2	75-98-9	pivalic acid	3
	102,0681	C5H10O2	108-21-4	isopropyl acetate	3
	102,0681	C5H10O2	109-52-4	valeric acid	3
	102,0681	C5H10O2	109-60-4	propyl acetate	3
	102,0681	C5H10O2	505-65-7	1,3-dioxepane	3
	102,0681	C5H10O2	97-99-4	tetrahydrofurfuryl alcohol	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	102,0681	C5H10O2	116-53-0	2-methylbutyric acid	3
	102,0681	C5H10O2	503-74-2	isovaleric acid	3
	110,1096	C8H14	931-87-3	(Z)-cyclooctene	3
	110,1096	C8H14	3710-30-3	octa-1,7-diene	3
	115,0633	C5H9NO2	4394-85-8	N-Formylmorpholine	3
	115,0633	C5H9NO2	147-85-3	L-proline	3
	115,0633	C5H9NO2	923-02-4	N-(hydroxymethyl)methacrylamide	3
	115,0633	C5H9NO2	14205-39-1	methyl 3-aminocrotonate	3
	120,0423	C4H8O4	19757-97-2	Methyl hydroxymethoxyacetate	3
	120,0575	C8H8O	96-09-3	(epoxyethyl)benzene	3
	120,0575	C8H8O	98-86-2	acetophenone	3
	120,0939	C9H12	98-82-8	Isopropylbenzol	3
	120,0939	C9H12	95-63-6	1,2,4-trimethylbenzene	3
	120,0939	C9H12	108-67-8	mesitylene	3
	120,0939	C9H12	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3
	120,0939	C9H12	3048-64-4	5-vinylnorborn-2-ene	3
	126,0429	C5H6N2O2	4866-00-6	4-methyloxazole-5-carboxamide	3
	128,0586	C5H8N2O2	77-71-4		3
	131,0946	C6H13NO2	61-90-5	L-leucine	3
	131,0946	C6H13NO2	622-40-2	2-morpholinoethanol	3
	132,0939	C10H12	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3
	132,0939	C10H12	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	132,0939	C10H12	768-56-9	4-phenylbut-1-ene	3
	134,0732	C9H10O	93-55-0	propiophenone	3
	134,0732	C9H10O	104-54-1	cinnamyl alcohol	3
	134,1096	C10H14	95-93-2		3
	134,1096	C10H14	527-53-7		3
	134,1096	C10H14	99-87-6	p-cymene	3
	134,1096	C10H14	4488-57-7	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	3
	134,1096	C10H14	25340-17-4	diethylbenzene	3
	134,1096	C10H14	68411-44-9	Benzene, butyl-, branched and linear	3
	134,1096	C10H14	105-05-5	1,4-diethylbenzene	3
	135,0545	C5H5N5	73-24-5	adenine	3
	143,0946	C7H13NO2	7747-35-5	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	3
	143,0946	C7H13NO2	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	143,9743	C2H6ClO3P	16672-87-0	Ethephon	3
	147,0718	C6H13NOS	141-98-0	O-isopropyl ethylthiocarbamate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	148,016	C8H4O3	85-44-9	phthalic anhydride	3
	148,0524	C9H8O2	621-82-9	cinnamic acid	3
	152,0334	C5H4N4O2	69-89-6	xanthine	3
	152,0334	C5H4N4O2	2465-59-0	oxypurinol	3
	154,0611	C6H7N3O2	86490-48-4	nitrophenylhydrazine	3
	158,0844	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	158,0844	C10H10N2	479-27-6	1,8-naphthylenediamine	3
	158,1096	C12H14	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	158,1096	C12H14	3748-13-8	m-bis(1-methylvinyl)benzene	3
	161,1052	C7H15NO3	541-15-1	Levocarnitin	3
	161,1056	C6H19NSi2	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	162,0317	C9H6O3	93-35-6	7-hydroxycoumarine	3
	162,1409	C12H18	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	162,1409	C12H18	7397-06-0		3
	162,1409	C12H18	4904-61-4	cyclododeca-1,5,9-triene	3
	162,1409	C12H18	99-62-7	1,3-diisopropylbenzene	3
	162,1409	C12H18	100-18-5	1,4-diisopropylbenzene	3
	162,1409	C12H18	25321-09-9	diisopropylbenzene	3
	164,0473	C9H8O3	156-06-9	phenylpyruvic acid	3
	164,0473	C9H8O3	15206-55-0	methyl benzoylformate	3
	164,1201	C11H16O	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	164,1201	C11H16O	88-60-8	6-tert-butyl-m-cresol	3
	164,1201	C11H16O	2409-55-4	2-tert-butyl-p-cresol	3
	164,1201	C11H16O	583-03-9	fenipentol	3
	165,079	C9H11NO2	94-09-7	benzocaine	3
	165,079	C9H11NO2	51-66-1	methacetin	3
	165,079	C9H11NO2	1129-41-5	Metolcarb	3
	165,079	C9H11NO2	938-73-8	Ethenzamide	3
	165,079	C9H11NO2	18595-18-1	Benzoic acid, 3-amino-4-methyl-, methyl ester	3
	165,079	C9H11NO2	24461-61-8	methyl (R)-aminophenylacetate	3
	166,063	C9H10O3	120-47-8	ethyl 4-hydroxybenzoate	3
	166,063	C9H10O3	121-32-4	ethyl vanillin	3
	166,063	C9H10O3	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3
	166,063	C9H10O3	11070-44-3	tetrahydromethylphthalic anhydride	3
	166,063	C9H10O3	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	6161-65-5	2-methoxy-6-methylbenzoic acid	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	180,0423	C9H8O4	50-78-2	acetylsalicyl acid	3
	182,0732	C13H10O	119-61-9	benzophenone	3
	182,0732	C13H10O	3218-36-8	p-phenylbenzaldehyde	3
	188,1565	C14H20	1203-17-4	1,1,2,3,3-pentamethylindan	3
	190,1358	C13H18O	125109-85-5	ß-methyl-3-(1-methylethyl)benzenepropanal	3
	190,1358	C13H18O	103-95-7	3-p-cumenyl-2-methylpropionaldehyde	3
	190,1358	C13H18O	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	3
	193,1103	C11H15NO2	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	193,1103	C11H15NO2	94-25-7	butamben	3
	193,1103	C11H15NO2	42542-10-9	3,4-methylenedioxymethamphetamine	3
	193,1103	C11H15NO2	1795-96-6	phenylalanine, ethyl ester	3
	193,1103	C11H15NO2	7298-73-9	N-Methylphenacetine	3
	193,1103	C11H15NO2	2631-40-5	Isoprocarb	3
	193,1103	C11H15NO2	2686-99-9	3,4,5-Trimethacarb	3
	193,1103	C11H15NO2	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	193,1103	C11H15NO2	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	194,0943	C11H14O3	94-26-8	Butyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	614-45-9	tert-butyl perbenzoate	3
	198,162	C12H22O2	111-81-9	methyl undec-10-enoate	3
	198,162	C12H22O2	688-84-6	2-ethylhexyl methacrylate	3
	198,162	C12H22O2	51000-52-3	vinyl neodecanoate	3
	198,162	C12H22O2		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	198,162	C12H22O2	89-48-5	menthyl acetate	3
	198,162	C12H22O2	150-84-5	citronellyl acetate	3
	198,162	C12H22O2	713-95-1	dodecan-5-olide	3
	198,162	C12H22O2	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	198,162	C12H22O2	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	203,1162	C8H21NOSi2	10416-59-8	trimethylsilyl N-trimethylsilylacetamidate	3
	204,115	C13H16O2	947-19-3	Methanone, Irgacure 184	3
	204,115	C13H16O2	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	204,115	C13H16O2	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	204,1514	C14H20O	80-54-6	Bucinal	3
	204,1514	C14H20O	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	206,1307	C13H18O2	15687-27-1	Ibuprofen	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	206,1307	C13H18O2	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	208,0524	C14H8O2	84-65-1	anthrachinone	3
	208,0524	C14H8O2	635-12-1	Anthracen-1,4-dione	3
	210,1021	C8H19O4P		Di-tert-butyl hydrogen phosphate	3
	210,1984	C14H26O		Degradation-Product	3
	210,1984	C14H26O	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	220,1463	C14H20O2	719-22-2	2,6-Di-tert-butylquinone	3
	227,1885	C13H25NO2		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	234,1256	C14H18O3	49763-96-4	stiripentol	3
	234,162	C15H22O2	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	234,162	C15H22O2	5444-75-7	2-ethylhexyl benzoate	3
	234,1984	C16H26O	54464-57-2	OTNE	3
	234,1984	C16H26O	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O		Degradation-Product	3
	234,1984	C16H26O	68155-66-8		3
	234,1984	C16H26O	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	234,1984	C16H26O	121158-58-5	Phenol, dodecyl-, branched	3
	236,1776	C15H24O2	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	240,1514	C17H20O	15087-24-8	3-benzylidenecamphor	3
	241,277	C16H35N	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	241,277	C16H35N	112-75-4	dimethyl(tetradecyl)amine	3
	241,277	C16H35N	1120-48-5	dioctylamine	3
	242,0903	C10H14N2O5	3424-98-4	Telbivudine	3
	242,0903	C10H14N2O5	50-89-5	thymidine	3
	242,2035	C18H26	1087-02-1	p-Dicyclohexylbenzene	3
	244,1787	C12H24N2O3	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	246,162	C16H22O2		Degradation-Product	3
	246,2348	C18H30	2719-62-2	6-Phenyldodecane	3
	246,2348	C18H30	25265-78-5	tetrapropylenebenzene	3
	248,1042	C6H20N2O6S	5080-22-8	N-isopropylhydroxylamine	3
	248,1049	C14H16O4	5292-53-5	diethyl (phenylmethylene)malonate	3
	248,1412	C15H20O3	71617-10-2	isopentyl p-methoxycinnamate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	248,1776	C16H24O2	18017-73-7	10-Phenyldecanoic acid	3
	248,1776	C16H24O2	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	250,1933	C16H26O2		Degradation-Product	3
	250,1933	C16H26O2	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	250,1933	C16H26O2	79-74-3	2,5-di-tert-pentylhydroquinone	3
	252,2089	C16H28O2	30507-70-1	(Z,E)-tetradeca-9,12-dienyl acetate	3
	253,2406	C16H31NO	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	253,2406	C16H31NO	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	254,2246	C16H30O2	142-90-5	dodecyl methacrylate	3
	258,1984	C18H26O	1222-05-5	Galaxolide	3
	258,1984	C18H26O		1-(4-(trans-4-butylcyclohexyl)phenyl)ethanone	3
	260,0507	C14H12O3S	33005-95-7	tiaprofenic acid	3
	260,1776	C17H24O2		Degradation-Product	3
	262,2297	C18H30O	5892-47-7	2,4,6-tri-sec-butylphenol	3
	265,1678	C15H23NO3	6452-71-7	oxprenolol	3
	266,1552	C12H26O4S		dodecyl sulfuric acid	3
	266,1552	C12H26O4S		2-butyloctyl-sulfonic acid	3
	266,1647	C12H27O4P	126-73-8	tributyl phosphate	3
	266,1647	C12H27O4P	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	266,261	C18H34O		Degradation-Product	3
	267,0968	C10H13N5O4	58-61-7	adenosine	3
	267,0968	C10H13N5O4	30516-87-1	Zidovudine	3
	268,2402	C17H32O2	21643-42-5	tetradecyl acrylate	3
	269,3083	C18H39N	112-69-6	hexadecyldimethylamine	3
	269,3083	C18H39N	124-30-1	octadecylamine	3
	272,0789	C9H13ClN6O2	42471-28-3	nimustine	3
	272,1776	C18H24O2	50-28-2	17-beta-Estradiol	3
	272,1776	C18H24O2	57-91-0	alfatradiol	3
	274,1933	C18H26O2	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	274,1933	C18H26O2	434-22-0	nandrolone	3
	276,1725	C17H24O3	456-59-7	cyclandelate	3
	276,1725	C17H24O3	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	276,2121	C14H32O3Si	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	3
	276,2121	C14H32O3Si	2943-75-1	triethoxyoctylsilane	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	277,1699	C19H21N2	524-81-2	mebhydroline	3
	278,1518	C16H22O4	84-74-2	Dibutyl phthalate	3
	278,1518	C16H22O4	84-69-5	diisobutyl phthalate	3
	278,1518	C16H22O4	1962-75-0	dibutyl terephthalate	3
	278,1882	C17H26O3	3115-49-9	4-nonylphenoxy acetic acid (NPE1C)	3
	278,2246	C18H30O2		Di-nonylpheno	3
	278,2246	C18H30O2		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	278,2246	C18H30O2	506-26-3	gamolenic acid	3
	280,2402	C18H32O2	60-33-3	linoleic acid	3
	281,2719	C18H35NO	1593-77-7	Dodemorph	3
	282,2559	C18H34O2	112-80-1	Oleic acid	3
	282,2559	C18H34O2	2549-53-3	tetradecyl methacrylate	3
	283,2875	C18H37NO	124-26-5	stearamide	3
	284,214	C20H28O	52-76-6	lynestrenol	3
	284,2351	C17H32O3		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	286,1933	C19H26O2	63-05-8	Androstendion	3
	286,1933	C19H26O2	846-48-0	boldenone	3
	286,2297	C20H30O	68-26-8	retinol	3
	288,2089	C19H28O2	481-30-1	Epitestosterone	3
	288,2089	C19H28O2	58-22-0	Testosterone	3
	288,2089	C19H28O2	53-43-0	prasterone	3
	288,2089	C19H28O2	1091-93-6	3-methoxyestra-2,5(10)-dien-17?-ol	3
	290,1882	C18H26O3	5466-77-3	Ethylhexyl methoxycinnamate	3
	290,2246	C19H30O2	521-18-6	androstanolone	3
	292,2038	C18H28O3	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	292,2766	C20H36O	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	294,2195	C18H30O3	2315-61-9	4-Octylphenol di-ethoxylate	3
	294,2216	C21H28N	57982-78-2	budipine	3
	298,1933	C20H26O2	68-22-4	Norethisteron	3
	298,2508	C18H34O3	13040-19-2	diricinoleate	3
	299,1521	C18H21NO3	125-29-1	Hydrocodone	3
	299,1521	C18H21NO3	76-57-3	codeine	3
	299,1521	C18H21NO3	968-46-7	deanol benzilate	3
	300,2664	C18H36O3	106-14-9	12-hydroxystearic acid	3
	301,2406	C20H31NO	144-11-6	trihexyphenidyl	3
	302,2246	C20H30O2	58-18-4	17-alpha-Methyltestosterone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	302,2246	C20H30O2	153-00-4	metenolone	3
	302,2457	C17H34O4	6731-36-8	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	3
	304,2402	C20H32O2	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	304,2402	C20H32O2	1424-00-6	mesterolone	3
	308,2351	C19H32O3	20427-84-3	4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group)	3
	309,2668	C19H35NO2	77-19-0	dicyclomine	3
	310,2297	C22H30O	54024-22-5	Desogestrel	3
	310,2508	C19H34O3	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	312,195	C18H24N4O	109889-09-0	granisetron	3
	314,155	C19H23ClN2	303-49-1	clomipramine	3
	314,2457	C18H34O4	109-43-3	dibutyl sebacate	3
	314,2457	C18H34O4	110-33-8	dihexyl adipate	3
	314,2457	C18H34O4	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	314,2457	C18H34O4	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	314,2457	C18H34O4	871-70-5	1,18-octadecanedioic acid	3
	316,2038	C20H28O3	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	316,2038	C20H28O3	2137-18-0	gestonorone	3
	320,2351	C20H32O3		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3
	320,2385	C17H36O3S	111360-16-8	2-hexyldecyl mesylate	3
	322,2144	C19H30O4	106807-78-7	2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C)	3
	327,3137	C20H41NO2	111-57-9	N-(2-hydroxyethyl)stearamide	3
	328,2402	C22H32O2	127-47-9	retinyl acetate	3
	328,2614	C19H36O4	56519-71-2	propane-1,3-diyl dioctanoate	3
	330,1831	C20H26O4	84-61-7	dicyclohexyl phthalate	3
	333,1608	C18H24ClN3O	119168-77-3	Tebufenpyrad	3
	333,1608	C18H24ClN3O	125225-28-7	Ipconazole	3
	333,2304	C20H31NO3	77-23-6	carbetapentane	3
	334,1441	C16FH19N4O3	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	335,1764	C18H26ClN3O	118-42-3	Hydroxychloroquine	3
	336,2512	C17H36O6	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	337,3345	C22H43NO		docos-13-enamide, Amides, C22 (unsaturated)	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	338,1882	C22H26O3	10453-86-8	Resmethrin	3
	338,2457	C20H34O4	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	340,1899	C19H24N4O2	100-33-4	Pentamidine	3
	340,1907	C21H26NO3	53-46-3	Methanthelinium	3
	340,2038	C22H28O3	51-98-9	Norethisterone acetate	3
	340,2038	C22H28O3	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	340,2038	C22H28O3	976-71-6	canrenone	3
	342,1831	C21H26O4	96609-16-4	lifibrol	3
	342,1852	C24H23NO	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	342,2195	C22H30O3	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	342,2195	C22H30O3	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	342,2559	C23H34O2	7069-42-3	retinyl propionate	3
	342,277	C20H38O4	762-12-9	bisdecanoyl peroxide	3
	342,277	C20H38O4	2915-57-3	bis(2-ethylhexyl) succinate	3
	342,2882	C19H38N2O3	4292-10-8	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	3
	344,2351	C22H32O3	434-05-9	Metenolone acetate	3
	344,2351	C22H32O3	520-85-4	Medroxyprogesteron	3
	344,2351	C22H32O3	2668-66-8	medrysone	3
	350,1158	C20H22O2Si2		Degradation-Product	3
	352,225	C20H32O5	363-24-6	dinoprostone	3
	352,225	C20H32O5	35121-78-9	epoprostenol	3
	353,293	C21H39NO3	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3
	354,2056	C20H26N4O2	3811-75-4	Hexamidine	3
	354,2064	C22H28NO3	125-51-9	pipenzolate	3
	354,2076	C16H34O6S		2-(2-dodecyloxyethoxy)ethyl sulfonic acid	3
	354,3134	C22H42O3		(3S,4S)-3-hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone	3
	356,2927	C21H40O4	28510-23-8	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	3
	356,2927	C21H40O4	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	358,3083	C21H42O4	31566-31-1	stearic acid, monoester with glycerol	3
	359,246	C22H33NO3	139-62-8	cyclomethycaine	3
	360,2301	C22H32O4	8003-24-5	4-methoxy-3-tert-butylphenol	3
	360,2301	C22H32O4	78919-13-8	Iloprost	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	366,0913	C15H21Cl2FN2O3	81406-37-3	Fluroxypyr-meptyl	3
	366,2195	C24H30O3	67392-87-4	drospirenone	3
	370,3083	C22H42O4	103-23-1	bis(2-ethylhexyl) adipate	3
	370,3083	C22H42O4	1330-86-5	diisooctyl adipate	3
	374,2093	C22H30O5	1172-63-0	Jasmolin II	3
	374,2093	C22H30O5	83-43-2	Methylprednisolone	3
	380,1042	C17H20N2O6S	61-32-5	Methicillin	3
	388,1886	C22H28O6	76-78-8	Quassin	3
	388,1899	C23H24N4O2		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	390,277	C24H38O4	117-84-0	Di-n-octylphthalate (DOP)	3
	390,277	C24H38O4	117-81-7	DEHP	3
	390,277	C24H38O4	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	390,277	C24H38O4	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	392,222	C25H30NO3	10405-02-4	Trospium	3
	398,2433	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	3
	399,1628	C18H26FN3O4S		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	400,3341	C27H44O2	41294-56-8	alphacalcidol	3
	402,2254	C20H34O8	77-90-7	Tributylacetylcitrate	3
	404,1195	C23H20N2O3S	57-96-5	sulfinpyrazone	3
	410,1905	C22H28F2O5	2135-17-3	flumetasone	3
	410,1905	C22H28F2O5	2557-49-5	diflorasone	3
	412,3553	C25H48O4	103-24-2	bis(2-ethylhexyl) azelate	3
	415,2723	C25H37NO4	155206-00-1	Bimatoprost	3
	415,2723	C25H37NO4	89365-50-4	Salmeterol	3
	418,3083	C26H42O4	28553-12-0	Diisononyl phthalate (DINP)	3
	422,3032	C25H42O5	1448-36-8	methyl cholate	3
	430,3083	C27H42O4	472-11-7	ruscogenin	3
	440,2345	C22H36N2O5S	144494-65-5	tirofiban	3
	467,3036	C29H41NO4	52485-79-7	Buprenorphin	3
	475,2723	C30H37NO4	126784-99-4	Ulipristal acetate	3
	499,304	BC21H45O12	30989-05-0	tris[2-[2-(2-methoxyethoxy)ethoxy]ethyl] orthoborate	3
	501,2879	C32H39NO4	83799-24-0	fexofenadine	3
	515,2917	C26H45NO7S	81-24-3	taurocholic acid	3
	551,3934	C30H53N3O6	173334-57-1	aliskiren	3
	563,3012	C30H46NO7P	98048-97-6	Fosinopril	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	733,5622	C40H80NO8P	63-89-8	Colfosceril-Palminat	3
Vendace	59,0735	C3H9N	75-50-3	trimethylamine	3
	71,0735	C4H9N	123-75-1	pyrrolidine	3
	89,0477	C3H7NO2	625-51-4	N-(hydroxymethyl)acetamide	3
	89,0477	C3H7NO2	79-46-9	2-nitropropane	3
	89,0477	C3H7NO2	107-95-9	ß-alanine	3
	89,0477	C3H7NO2	108-03-2	1-nitropropane	3
	89,0477	C3H7NO2	107-97-1	sarcosine	3
	89,0477	C3H7NO2	56-41-7	L-alanine	3
	93,0578	C6H7N	62-53-3	Aniline	3
	93,0578	C6H7N	108-99-6	3-methylpyridine	3
	97,969	C2H4Cl2	75-34-3	1,1-Dichlorethan	3
	97,969	C2H4Cl2	107-06-2	1,2-dichloroethane	3
	103,0997	C5H13NO	3179-63-3	3-dimethylaminopropan-1-ol	3
	103,0997	C5H13NO	108-16-7	1-(dimethylamino)propan-2-ol	3
	103,0997	C5H13NO	6291-85-6	3-ethoxypropylamine	3
	104,0626	C8H8	100-42-5	Styrene	3
	110,1096	C8H14	931-87-3	(Z)-cyclooctene	3
	110,1096	C8H14	3710-30-3	octa-1,7-diene	3
	111,0433	C4H5N3O	71-30-7	cytosine	3
	115,0633	C5H9NO2	4394-85-8	N-Formylmorpholine	3
	115,0633	C5H9NO2	147-85-3	L-proline	3
	115,0633	C5H9NO2	923-02-4	N-(hydroxymethyl)methacrylamide	3
	115,0633	C5H9NO2	14205-39-1	methyl 3-aminocrotonate	3
	120,0423	C4H8O4	19757-97-2	Methyl hydroxymethoxyacetate	3
	120,0575	C8H8O	96-09-3	(epoxyethyl)benzene	3
	120,0575	C8H8O	98-86-2	acetophenone	3
	120,0939	C9H12	98-82-8	Isopropylbenzol	3
	120,0939	C9H12	95-63-6	1,2,4-trimethylbenzene	3
	120,0939	C9H12	108-67-8	mesitylene	3
	120,0939	C9H12	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3
	120,0939	C9H12	3048-64-4	5-vinylnorborn-2-ene	3
	125,0147	C2H7NO3S	107-35-7	taurine	3
	126,0429	C5H6N2O2	4866-00-6	4-methyloxazole-5-carboxamide	3
	126,1157	C7H14N2	5351-04-2	3-diethylaminopropiononitrile	3
	131,0946	C6H13NO2	61-90-5	L-leucine	3
	131,0946	C6H13NO2	622-40-2	2-morpholinoethanol	3
	132,0939	C10H12	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	132,0939	C10H12	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	132,0939	C10H12	768-56-9	4-phenylbut-1-ene	3
	135,0545	C5H5N5	73-24-5	adenine	3
	143,0946	C7H13NO2	7747-35-5	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	3
	143,0946	C7H13NO2	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	143,9743	C2H6ClO3P	16672-87-0	Ethephon	3
	147,0718	C6H13NOS	141-98-0	O-isopropyl ethylthiocarbamate	3
	148,016	C8H4O3	85-44-9	phthalic anhydride	3
	148,0524	C9H8O2	621-82-9	cinnamic acid	3
	152,0334	C5H4N4O2	69-89-6	xanthine	3
	152,0334	C5H4N4O2	2465-59-0	oxypurinol	3
	154,0611	C6H7N3O2	86490-48-4	nitrophenylhydrazine	3
	158,0844	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	158,0844	C10H10N2	479-27-6	1,8-naphthylenediamine	3
	158,1096	C12H14	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	158,1096	C12H14	3748-13-8	m-bis(1-methylvinyl)benzene	3
	161,1052	C7H15NO3	541-15-1	Levocarnitin	3
	161,1056	C6H19NSi2	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	162,0317	C9H6O3	93-35-6	7-hydroxycoumarine	3
	162,1409	C12H18	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	162,1409	C12H18	4904-61-4	cyclododeca-1,5,9-triene	3
	162,1409	C12H18	99-62-7	1,3-diisopropylbenzene	3
	162,1409	C12H18	100-18-5	1,4-diisopropylbenzene	3
	162,1409	C12H18	25321-09-9	diisopropylbenzene	3
	164,0473	C9H8O3	156-06-9	phenylpyruvic acid	3
	164,0473	C9H8O3	15206-55-0	methyl benzoylformate	3
	164,1201	C11H16O	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	164,1201	C11H16O	88-60-8	6-tert-butyl-m-cresol	3
	164,1201	C11H16O	2409-55-4	2-tert-butyl-p-cresol	3
	164,1201	C11H16O	583-03-9	fenipentol	3
	165,079	C9H11NO2	94-09-7	benzocaine	3
	165,079	C9H11NO2	51-66-1	methacetin	3
	165,079	C9H11NO2	1129-41-5	Metolcarb	3
	165,079	C9H11NO2	938-73-8	Ethenzamide	3
	165,079	C9H11NO2	18595-18-1	Benzoic acid, 3-amino-4-methyl-, methyl ester	3
	165,079	C9H11NO2	24461-61-8	methyl (R)-aminophenylacetate	3
	166,063	C9H10O3	120-47-8	ethyl 4-hydroxybenzoate	3
	166,063	C9H10O3	121-32-4	ethyl vanillin	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	166,063	C9H10O3	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3
	166,063	C9H10O3	11070-44-3	tetrahydromethylphthalic anhydride	3
	166,063	C9H10O3	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	170,0943	C9H14O3	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	170,0943	C9H14O3	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	180,0423	C9H8O4	50-78-2	acetylsalicyl acid	3
	182,0732	C13H10O	119-61-9	benzophenone	3
	182,0732	C13H10O	3218-36-8	p-phenylbenzaldehyde	3
	188,1565	C14H20	1203-17-4	1,1,2,3,3-pentamethylindan	3
	190,1358	C13H18O	125109-85-5	ß-methyl-3-(1-methylethyl)benzenepropanal	3
	190,1358	C13H18O	103-95-7	3-p-cumenyl-2-methylpropionaldehyde	3
	190,1358	C13H18O	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	3
	193,1103	C11H15NO2	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	193,1103	C11H15NO2	94-25-7	butamben	3
	193,1103	C11H15NO2	42542-10-9	3,4-methylenedioxymethamphetamine	3
	193,1103	C11H15NO2	1795-96-6	phenylalanine, ethyl ester	3
	193,1103	C11H15NO2	7298-73-9	N-Methylphenacetine	3
	193,1103	C11H15NO2	2631-40-5	Isoprocarb	3
	193,1103	C11H15NO2	2686-99-9	3,4,5-Trimethacarb	3
	193,1103	C11H15NO2	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	193,1103	C11H15NO2	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	194,0943	C11H14O3	94-26-8	Butyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	614-45-9	tert-butyl perbenzoate	3
	198,162	C12H22O2	111-81-9	methyl undec-10-enoate	3
	198,162	C12H22O2	688-84-6	2-ethylhexyl methacrylate	3
	198,162	C12H22O2	51000-52-3	vinyl neodecanoate	3
	198,162	C12H22O2		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	198,162	C12H22O2	89-48-5	menthyl acetate	3
	198,162	C12H22O2	150-84-5	citronellyl acetate	3
	198,162	C12H22O2	713-95-1	dodecan-5-olide	3
	198,162	C12H22O2	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	198,162	C12H22O2	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	204,115	C13H16O2	947-19-3	Methanone, Irgacure 184	3
	204,115	C13H16O2	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	204,115	C13H16O2	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	204,1514	C14H20O	80-54-6	Bucinal	3
	204,1514	C14H20O	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	206,1307	C13H18O2	15687-27-1	Ibuprofen	3
	206,1307	C13H18O2	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	208,0524	C14H8O2	84-65-1	anthrachinone	3
	208,0524	C14H8O2	635-12-1	Anthracen-1,4-dione	3
	210,1021	C8H19O4P		Di-tert-butyl hydrogen phosphate	3
	220,1463	C14H20O2	719-22-2	2,6-Di-tert-butylquinone	3
	227,1885	C13H25NO2		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	234,162	C15H22O2	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	234,162	C15H22O2	5444-75-7	2-ethylhexyl benzoate	3
	234,1984	C16H26O	54464-57-2	OTNE	3
	234,1984	C16H26O	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O		Degradation-Product	3
	234,1984	C16H26O	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	234,1984	C16H26O	121158-58-5	Phenol, dodecyl-, branched	3
	236,1776	C15H24O2	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	241,277	C16H35N	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	241,277	C16H35N	112-75-4	dimethyl(tetradecyl)amine	3
	241,277	C16H35N	1120-48-5	dioctylamine	3
	242,2035	C18H26	1087-02-1	p-Dicyclohexylbenzene	3
	246,162	C16H22O2		Degradation-Product	3
	246,2348	C18H30	2719-62-2	6-Phenyldodecane	3
	246,2348	C18H30	25265-78-5	tetrapropylenebenzene	3
	248,1042	C6H20N2O6S	5080-22-8	N-isopropylhydroxylamine	3
	248,1049	C14H16O4	5292-53-5	diethyl (phenylmethylene)malonate	3
	248,1412	C15H20O3	71617-10-2	isopentyl p-methoxycinnamate	3
	248,1776	C16H24O2	18017-73-7	10-Phenyldecanoic acid	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	248,1776	C16H24O2	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	250,1933	C16H26O2		Degradation-Product	3
	250,1933	C16H26O2	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	250,1933	C16H26O2	79-74-3	2,5-di-tert-pentylhydroquinone	3
	251,1644	C15H22O3		gemfibrozil	2
	253,2406	C16H31NO	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	253,2406	C16H31NO	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	254,2246	C16H30O2	142-90-5	dodecyl methacrylate	3
	258,1984	C18H26O	1222-05-5	Galaxolide	3
	260,0507	C14H12O3S	33005-95-7	tiaprofenic acid	3
	262,2297	C18H30O	5892-47-7	2,4,6-tri-sec-butylphenol	3
	265,1678	C15H23NO3	6452-71-7	oxprenolol	3
	266,1552	C12H26O4S		dodecyl sulfuric acid	3
	266,1552	C12H26O4S		2-butyloctyl-sulfonic acid	3
	266,1647	C12H27O4P	126-73-8	tributyl phosphate	3
	266,1647	C12H27O4P	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	266,1882	C16H26O3	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	266,1882	C16H26O3	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	266,261	C18H34O		Degradation-Product	3
	267,0968	C10H13N5O4	58-61-7	adenosine	3
	267,0968	C10H13N5O4	30516-87-1	Zidovudine	3
	268,2402	C17H32O2	21643-42-5	tetradecyl acrylate	3
	269,3083	C18H39N	112-69-6	hexadecyldimethylamine	3
	269,3083	C18H39N	124-30-1	octadecylamine	3
	272,0789	C9H13ClN6O2	42471-28-3	nimustine	3
	272,1776	C18H24O2	50-28-2	17-beta-Estradiol	3
	272,1776	C18H24O2	57-91-0	alfatradiol	3
	274,1933	C18H26O2	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	274,1933	C18H26O2	434-22-0	nandrolone	3
	276,1725	C17H24O3	456-59-7	cyclandelate	3
	276,1725	C17H24O3	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	277,1699	C19H21N2	524-81-2	mebhydroline	3
	278,1518	C16H22O4	84-74-2	Dibutyl phthalate	3
	278,1518	C16H22O4	84-69-5	diisobutyl phthalate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	278,1518	C16H22O4	1962-75-0	dibutyl terephthalate	3
	278,1882	C17H26O3	3115-49-9	4-nonylphenoxy acetic acid (NPE1C)	3
	278,2246	C18H30O2		Di-nonylpheno	3
	278,2246	C18H30O2		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	278,2246	C18H30O2	506-26-3	gamolenic acid	3
	280,2402	C18H32O2	60-33-3	linoleic acid	3
	281,2719	C18H35NO	1593-77-7	Dodemorph	3
	282,2559	C18H34O2	112-80-1	Oleic acid	3
	282,2559	C18H34O2	2549-53-3	tetradecyl methacrylate	3
	283,2875	C18H37NO	124-26-5	stearamide	3
	284,214	C20H28O	52-76-6	lynestrenol	3
	284,2351	C17H32O3		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	286,1933	C19H26O2	63-05-8	Androstendion	3
	286,1933	C19H26O2	846-48-0	boldenone	3
	286,2144	C16H30O4	6846-50-0	TXIB	3
	286,2144	C16H30O4	7491-02-3	diisopropyl sebacate	3
	286,2297	C20H30O	68-26-8	retinol	3
	288,2089	C19H28O2	481-30-1	Epitestosterone	3
	288,2089	C19H28O2	58-22-0	Testosterone	3
	288,2089	C19H28O2	53-43-0	prasterone	3
	288,2089	C19H28O2	1091-93-6	3-methoxyestra-2,5(10)-dien-17?-ol	3
	290,1882	C18H26O3	5466-77-3	Ethylhexyl methoxycinnamate	3
	292,2038	C18H28O3	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	292,2766	C20H36O	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	294,2195	C18H30O3	2315-61-9	4-Octylphenol di-ethoxylate	3
	294,2216	C21H28N	57982-78-2	budipine	3
	297,2668	C18H35NO2	118134-30-8	Spiroxamine	3
	298,1933	C20H26O2	68-22-4	Norethisteron	3
	298,2508	C18H34O3	13040-19-2	diricinoleate	3
	299,1521	C18H21NO3	125-29-1	Hydrocodone	3
	299,1521	C18H21NO3	76-57-3	codeine	3
	299,1521	C18H21NO3	968-46-7	deanol benzilate	3
	300,2089	C20H28O2	5300-03-8	Alitretinoin	3
	300,2089	C20H28O2	1740-19-8	Abieta-8,11,13-trien-18-oic acid	3
	300,2089	C20H28O2	4759-48-2	Isotretinoin	3
	300,2089	C20H28O2	57144-06-6	3-methoxyandrosta-3,5-dien-17-one	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	300,2664	C18H36O3	106-14-9	12-hydroxystearic acid	3
	301,2406	C20H31NO	144-11-6	trihexyphenidyl	3
	302,1882	C19H26O3	584-79-2	(RS)-3-allyl-2-methyl-4-oxocyclopent-2-enyl-(1RS,3RS;1RS,3SR)-2,2-dimethyl-3-(2-methylprop-1-enyl)-cyclopropanecarboxylate (all isomers; ratio: 1:1:1:1:1:1:1:1)	3
	302,1882	C19H26O3	560-62-3	Androst-4-ene-3,17-dione, 9-hydroxy-	3
	302,1882	C19H26O3	566-48-3	formestane	3
	302,2246	C20H30O2	58-18-4	17-alpha-Methyltestosterone	3
	302,2246	C20H30O2	153-00-4	metenolone	3
	302,2457	C17H34O4	6731-36-8	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	3
	304,2402	C20H32O2	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	304,2402	C20H32O2	1424-00-6	mesterolone	3
	309,2668	C19H35NO2	77-19-0	dicyclomine	3
	310,2297	C22H30O	54024-22-5	Desogestrel	3
	310,2508	C19H34O3	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	312,195	C18H24N4O	109889-09-0	granisetron	3
	314,155	C19H23ClN2	303-49-1	clomipramine	3
	314,2246	C21H30O2	13956-29-1	cannabidiol	3
	314,2246	C21H30O2	1972-08-3	delta(9)-tetrahydrocannabinol	3
	314,2246	C21H30O2	57-83-0	Progesteron	3
	314,2246	C21H30O2	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	314,2457	C18H34O4	109-43-3	dibutyl sebacate	3
	314,2457	C18H34O4	110-33-8	dihexyl adipate	3
	314,2457	C18H34O4	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	314,2457	C18H34O4	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	314,2457	C18H34O4	871-70-5	1,18-octadecanedioic acid	3
	316,2038	C20H28O3	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	316,2038	C20H28O3	2137-18-0	gestonorone	3
	320,2351	C20H32O3		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3
	320,2385	C17H36O3S	111360-16-8	2-hexyldecyl mesylate	3
	322,2144	C19H30O4	106807-78-7	2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C)	3
	326,2402	C18H35AlO3	13419-15-3	(octadecanoato-O)oxoaluminium	3
	327,3137	C20H41NO2	111-57-9	N-(2-hydroxyethyl)stearamide	3
	328,2402	C22H32O2	127-47-9	retinyl acetate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	328,2614	C19H36O4	56519-71-2	propane-1,3-diyl dioctanoate	3
	330,1831	C20H26O4	84-61-7	dicyclohexyl phthalate	3
	333,1608	C18H24ClN3O	119168-77-3	Tebufenpyrad	3
	333,1608	C18H24ClN3O	125225-28-7	Ipconazole	3
	333,2304	C20H31NO3	77-23-6	carbetapentane	3
	334,1441	C16FH19N4O3	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	335,1764	C18H26ClN3O	118-42-3	Hydroxychloroquine	3
	336,2512	C17H36O6	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	337,3345	C22H43NO		docos-13-enamide, Amides, C22 (unsaturated)	3
	338,1882	C22H26O3	10453-86-8	Resmethrin	3
	338,2457	C20H34O4	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	340,1899	C19H24N4O2	100-33-4	Pentamidine	3
	340,1907	C21H26NO3	53-46-3	Methanthelinium	3
	340,2038	C22H28O3	51-98-9	Norethisterone acetate	3
	340,2038	C22H28O3	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	340,2038	C22H28O3	976-71-6	canrenone	3
	342,1852	C24H23NO	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	342,2195	C22H30O3	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	342,2195	C22H30O3	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	342,2559	C23H34O2	7069-42-3	retinyl propionate	3
	342,277	C20H38O4	762-12-9	bisdecanoyl peroxide	3
	342,277	C20H38O4	2915-57-3	bis(2-ethylhexyl) succinate	3
	342,2882	C19H38N2O3	4292-10-8	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	3
	344,2351	C22H32O3	434-05-9	Metenolone acetate	3
	344,2351	C22H32O3	520-85-4	Medroxyprogesteron	3
	344,2351	C22H32O3	2668-66-8	medrysone	3
	350,1158	C20H22O2Si2		Degradation-Product	3
	352,225	C20H32O5	363-24-6	dinoprostone	3
	352,225	C20H32O5	35121-78-9	epoprostenol	3
	354,2056	C20H26N4O2	3811-75-4	Hexamidine	3
	354,2064	C22H28NO3	125-51-9	pipenzolate	3
	354,2076	C16H34O6S		2-(2-dodecyloxyethoxy)ethyl sulfonic acid	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	354,3134	C22H42O3		(3S,4S)-3-hexyl-4-[(R)-2-hydroxytridecyl]-2-oxetanone	3
	356,2927	C21H40O4	28510-23-8	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	3
	356,2927	C21H40O4	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	358,3083	C21H42O4	31566-31-1	stearic acid, monoester with glycerol	3
	359,246	C22H33NO3	139-62-8	cyclomethycaine	3
	360,2301	C22H32O4	8003-24-5	4-methoxy-3-tert-butylphenol	3
	360,2301	C22H32O4	78919-13-8	Iloprost	3
	366,0913	C15H21Cl2FN2O3	81406-37-3	Fluroxypyr-meptyl	3
	366,2195	C24H30O3	67392-87-4	drospirenone	3
	370,3083	C22H42O4	103-23-1	bis(2-ethylhexyl) adipate	3
	370,3083	C22H42O4	1330-86-5	diisooctyl adipate	3
	372,1937	C22H28O5	24916-90-3	9?,11?-epoxy-17,21-dihydroxy-16?-methylpregna-1,4-diene-3,20-dione	3
	372,1937	C22H28O5	599-33-7	prednylidene	3
	374,2093	C22H30O5	1172-63-0	Jasmolin II	3
	374,2093	C22H30O5	83-43-2	Methylprednisolone	3
	380,1042	C17H20N2O6S	61-32-5	Methicillin	3
	386,1729	C22H26O6	2618-77-1		3
	388,1899	C23H24N4O2		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	390,277	C24H38O4	117-84-0	Di-n-octylphthalate (DOP)	3
	390,277	C24H38O4	117-81-7	DEHP	3
	390,277	C24H38O4	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	390,277	C24H38O4	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	392,222	C25H30NO3	10405-02-4	Trospium	3
	392,2927	C24H40O4	474-25-9	chenodeoxycholic acid	3
	392,2927	C24H40O4	128-13-2	ursodeoxycholic acid	3
	394,2719	C23H38O5	64318-79-2	gemeprost	3
	398,2433	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	3
	399,1628	C18H26FN3O4S		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	400,3341	C27H44O2	41294-56-8	alphacalcidol	3
	402,2254	C20H34O8	77-90-7	Tributylacetylcitrate	3
	404,1195	C23H20N2O3S	57-96-5	sulfinpyrazone	3
	410,1905	C22H28F2O5	2135-17-3	flumetasone	3
	410,1905	C22H28F2O5	2557-49-5	diflorasone	3
	412,3553	C25H48O4	103-24-2	bis(2-ethylhexyl) azelate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	414,2042	C24H30O6	107724-20-9	eplerenone	3
	414,2042	C24H30O6		2,6-bis(4-ethylphenyl)perhydro-1,3,5,7-tetraoxanaphth-4-ylethane-1,2-diol	3
	415,2723	C25H37NO4	155206-00-1	Bimatoprost	3
	415,2723	C25H37NO4	89365-50-4	Salmeterol	3
	418,3083	C26H42O4	28553-12-0	Diisononyl phthalate (DINP)	3
	422,3032	C25H42O5	1448-36-8	methyl cholate	3
	430,3083	C27H42O4	472-11-7	ruscogenin	3
	467,3036	C29H41NO4	52485-79-7	Buprenorphin	3
	475,2723	C30H37NO4	126784-99-4	Ulipristal acetate	3
	501,2879	C32H39NO4	83799-24-0	fexofenadine	3
	551,3934	C30H53N3O6	173334-57-1	aliskiren	3
	563,3012	C30H46NO7P	98048-97-6	Fosinopril	3
	733,5622	C40H80NO8P	63-89-8	Colfosceril-Palminat	3
Brown Trout	59	C3H9N	75-31-0	isopropylamine	3
	71	C4H9N	123-75-1	pyrrolidine	3
	89	C3H7NO2	625-51-4	N-(hydroxymethyl)acetamide	3
	93	C6H7N	108-99-6	3-methylpyridine	3
	93	C6H7N	62-53-3	Aniline	3
	102	C5H10O2	116-53-0	2-methylbutyric acid	3
	102	C5H10O2	108-21-4	isopropyl acetate	3
	102	C5H10O2	503-74-2	isovaleric acid	3
	102	C5H10O2	75-98-9	pivalic acid	3
	102	C5H10O2	109-60-4	propyl acetate	3
	102	C5H10O2	109-52-4	valeric acid	3
	103	C5H13NO	108-16-7	1-(dimethylamino)propan-2-ol	3
	103	C5H13NO	3179-63-3	3-dimethylaminopropan-1-ol	3
	103	C5H13NO	6291-85-6	3-ethoxypropylamine	3
	110	C8H14	931-87-3	(Z)-cyclooctene	3
	110	C8H14	3710-30-3	octa-1,7-diene	3
	111	C4H5N3O	71-30-7	cytosine	3
	115	C5H9NO2	147-85-3	L-proline	3
	115	C5H9NO2	14205-39-1	methyl 3-aminocrotonate	3
	115	C5H9NO2	923-02-4	N-(hydroxymethyl)methacrylamide	3
	115	C5H9NO2	4394-85-8	N-Formylmorpholine	3
	120	C4H8O4	19757-97-2	Methyl hydroxymethoxyacetate	3
	120	C8H8O	96-09-3	(epoxyethyl)benzene	3
	120	C8H8O	98-86-2	acetophenone	3
	120	C9H12	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	120	C9H12	3048-64-4	5-vinylnorborn-2-ene	3
	120	C9H12	98-82-8	Isopropylbenzol	3
	120	C9H12	108-67-8	mesitylene	3
	125	C2H7NO3S	107-35-7	taurine	3
	132	C10H12	119-64-2	1,2,3,4-tetrahydronaphthalene	3
	132	C10H12	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	3
	132	C10H12	768-56-9	4-phenylbut-1-ene	3
	134	C10H14	4488-57-7	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	3
	134	C10H14	68411-44-9	Benzene, butyl-, branched and linear	3
	134	C10H14	25340-17-4	diethylbenzene	3
	134	C10H14	99-87-6	p-cymene	3
	136	C5H4N4O	315-30-0	allopurinol	3
	143	C7H13NO2	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	143	C7H13NO2	7747-35-5	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	3
	144	C2H6ClO3P	16672-87-0	Ethephon	3
	147	C6H13NOS	141-98-0	O-isopropyl ethylthiocarbamate	3
	148	C8H4O3	85-44-9	phthalic anhydride	3
	148	C9H8O2	621-82-9	cinnamic acid	3
	152	C5H4N4O2	2465-59-0	oxypurinol	3
	152	C5H4N4O2	69-89-6	xanthine	3
	152	C8H12N2O	2814-20-2	G27550	3
	154	C6H7N3O2	86490-48-4	nitrophenylhydrazine	3
	158	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	162	C9H6O3	93-35-6	7-hydroxycoumarine	3
	162	C12H18	4904-61-4	cyclododeca-1,5,9-triene	3
	162	C12H18	25321-09-9	diisopropylbenzene	3
	164	C9H8O3	15206-55-0	methyl benzoylformate	3
	164	C9H8O3	156-06-9	phenylpyruvic acid	3
	164	C11H16O	583-03-9	fenipentol	3
	165	C9H11NO2	94-09-7	benzocaine	3
	165	C9H11NO2	18595-18-1	Benzoic acid, 3-amino-4-methyl-, methyl ester	3
	165	C9H11NO2	938-73-8	Ethenzamide	3
	165	C9H11NO2	51-66-1	methacetin	3
	165	C9H11NO2	24461-61-8	methyl (R)-aminophenylacetate	3
	165	C9H11NO2	1129-41-5	Metolcarb	3
	166	C9H10O3	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	166	C9H10O3	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	166	C9H10O3	120-47-8	ethyl 4-hydroxybenzoate	3
	166	C9H10O3	121-32-4	ethyl vanillin	3
	166	C9H10O3	34090-76-1	tetrahydro-4-methylphthalic anhydride	3
	166	C9H10O3	11070-44-3	tetrahydromethylphthalic anhydride	3
	170	C9H14O3	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	170	C9H14O3	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	179	C6H17NO3Si	13822-56-5	3-(trimethoxysilyl)propylamine	3
	180	C9H8O4	50-78-2	acetylsalicyl acid	3
	182	C13H10O	119-61-9	benzophenone	3
	182	C13H10O	3218-36-8	p-phenylbenzaldehyde	3
	188	C14H20	1203-17-4	1,1,2,3,3-pentamethylindan	3
	190	C13H18O	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	3
	190	C13H18O	103-95-7	3-p-cumenyl-2-methylpropionaldehyde	3
	190	C13H18O	125109-85-5	ß-methyl-3-(1-methylethyl)benzenepropanal	3
	193	C11H15NO2	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	193	C11H15NO2	2686-99-9	3,4,5-Trimethacarb	3
	193	C11H15NO2	94-25-7	butamben	3
	193	C11H15NO2	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	193	C11H15NO2	2631-40-5	Isoprocarb	3
	193	C11H15NO2	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	193	C11H15NO2	7298-73-9	N-Methylphenacetine	3
	193	C11H15NO2	1795-96-6	phenylalanine, ethyl ester	3
	194	C11H14O3	94-26-8	Butyl 4-hydroxybenzoate	3
	194	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	3
	198	C12H22O2	688-84-6	2-ethylhexyl methacrylate	3
	198	C12H22O2	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	198	C12H22O2	150-84-5	citronellyl acetate	3
	198	C12H22O2	713-95-1	dodecan-5-olide	3
	198	C12H22O2		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	198	C12H22O2	89-48-5	menthyl acetate	3
	198	C12H22O2	111-81-9	methyl undec-10-enoate	3
	198	C12H22O2	51000-52-3	vinyl neodecanoate	3
	204	C13H16O2	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	204	C13H16O2	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	204	C13H16O2	947-19-3	Methanone, Irgacure 184	3
	204	C14H20O	80-54-6	Bucinal	3
	206	C13H18O2	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	210	C8H19O4P		Di-tert-butyl hydrogen phosphate	3
	210	C14H26O	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	220	C14H20O2	719-22-2	2,6-Di-tert-butylquinone	3
	227	C13H25NO2		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	234	C14H18O3	49763-96-4	stiripentol	3
	234	C15H22O2	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	234	C15H22O2	5444-75-7	2-ethylhexyl benzoate	3
	234	C16H26O	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	234	C16H26O	54464-57-2	OTNE	3
	234	C16H26O	121158-58-5	Phenol, dodecyl-, branched	3
	236	C15H24O2	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	3
	241	C16H35N	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	241	C16H35N	112-75-4	dimethyl(tetradecyl)amine	3
	241	C16H35N	1120-48-5	dioctylamine	3
	242	C10H14N2O5	3424-98-4	Telbivudine	3
	242	C10H14N2O5	50-89-5	thymidine	3
	244	C12H24N2O3	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	248	C6H20N2O6S	5080-22-8	N-isopropylhydroxylamine	3
	248	C14H16O4	5292-53-5	diethyl (phenylmethylene)malonate	3
	248	C15H20O3	71617-10-2	isopentyl p-methoxycinnamate	3
	248	C16H24O2	18017-73-7	10-Phenyldecanoic acid	3
	248	C16H24O2	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3
	250	C16H26O2	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	253	C16H31NO	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	253	C16H31NO	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	254	C16H30O2	142-90-5	dodecyl methacrylate	3
	258	C18H26O	1222-05-5	Galaxolide	3
	260	C14H12O3S	33005-95-7	tiaprofenic acid	3
	265	C15H23NO3	6452-71-7	oxprenolol	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	266	C18H18O2	13029-44-2	Dienestrol	3
	266	C18H18O2	517-09-9	Equilenin	3
	266	C18H18O2	63250-25-9	isopropyldibenzoylmethane	3
	266	C12H26O4S		2-butyloctyl-sulfonic acid	3
	266	C12H27O4P	126-73-8	tributyl phosphate	3
	266	C12H27O4P	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	266	C16H26O3	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	266	C16H26O3	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	267	C10H13N5O4	58-61-7	adenosine	3
	267	C10H13N5O4	30516-87-1	Zidovudine	3
	268	C17H32O2	21643-42-5	tetradecyl acrylate	3
	269	C18H39N	112-69-6	hexadecyldimethylamine	3
	269	C18H39N	124-30-1	octadecylamine	3
	272	C9H13ClN6O2	42471-28-3	nimustine	3
	272	C18H24O2	50-28-2	17-beta-Estradiol	3
	272	C18H24O2	57-91-0	alfatradiol	3
	274	C18H26O2	54406-48-3	1-ethynyl-2-methylpent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropa- necarboxylate	3
	278	C16H22O4	84-74-2	Dibutyl phthalate	3
	278	C16H22O4	1962-75-0	dibutyl terephthalate	3
	278	C16H22O4	84-69-5	diisobutyl phthalate	3
	278	C17H26O3	3115-49-9	4-nonylphenoxy acetic acid (NPE1C)	3
	278	C18H30O2		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	278	C18H30O2	506-26-3	gamolenic acid	3
	280	C18H32O2	60-33-3	linoleic acid	3
	281	C18H35NO	1593-77-7	Dodemorph	3
	282	C18H34O2	112-80-1	Oleic acid	3
	282	C18H34O2	2549-53-3	tetradecyl methacrylate	3
	283	C18H37NO	124-26-5	stearamide	3
	284	C20H28O	52-76-6	lynestrenol	3
	284	C17H32O3		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	286	C19H26O2	63-05-8	Androstendion	3
	286	C19H26O2	846-48-0	boldenone	3
	288	C19H28O2	1091-93-6	3-methoxyestra-2,5(10)-dien-17?-ol	3
	288	C19H28O2	481-30-1	Epitestosterone	3
	288	C19H28O2	53-43-0	prasterone	3
	288	C19H28O2	58-22-0	Testosterone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	290	C18H26O3	5466-77-3	Ethylhexyl methoxycinnamate	3
	292	C18H28O3	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	292	C20H36O	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	294	C18H30O3	2315-61-9	4-Octylphenol di-ethoxylate	3
	294	C21H28N	57982-78-2	budipine	3
	297	C18H35NO2	118134-30-8	Spiroxamine	3
	298	C20H26O2	68-22-4	Norethisteron	3
	299	C18H21NO3	76-57-3	codeine	3
	299	C18H21NO3	968-46-7	deanol benzilate	3
	299	C18H21NO3	125-29-1	Hydrocodone	3
	301	C20H31NO	144-11-6	trihexyphenidyl	3
	302	C19H26O3	560-62-3	Androst-4-ene-3,17-dione, 9-hydroxy-	3
	302	C19H26O3	566-48-3	formestane	3
	302	C20H30O2	58-18-4	17-alpha-Methyltestosterone	3
	302	C20H30O2	153-00-4	metenolone	3
	304	C20H32O2	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	304	C20H32O2	1424-00-6	mesterolone	3
	308	C19H32O3	20427-84-3	4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group)	3
	309	C19H35NO2	77-19-0	dicyclomine	3
	310	C22H30O	54024-22-5	Desogestrel	3
	314	C19H23ClN2	303-49-1	clomipramine	3
	314	C21H30O2	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	314	C21H30O2	57-83-0	Progesteron	3
	314	C18H34O4	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	314	C18H34O4	871-70-5	1,18-octadecanedioic acid	3
	314	C18H34O4	109-43-3	dibutyl sebacate	3
	314	C18H34O4	110-33-8	dihexyl adipate	3
	316	C20H28O3	25402-06-6	3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	3
	328	C19H36O4	56519-71-2	propane-1,3-diyl dioctanoate	3
	330	C20H26O4	84-61-7	dicyclohexyl phthalate	3
	333	C18H24ClN3O	125225-28-7	Ipconazole	3
	333	C18H24ClN3O	119168-77-3	Tebufenpyrad	3
	333	C20H31NO3	77-23-6	carbetapentane	3
	334	C16FH19N4O3	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
				oxo-1,6-dihydropyrimidine-4-carboxamide	
	335	C18H26ClN3O	118-42-3	Hydroxychloroquine	3
	336	C17H36O6	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	338	C22H26O3	10453-86-8	Resmethrin	3
	340	C19H24N4O2	100-33-4	Pentamidine	3
	340	C21H26NO3	53-46-3	Methanthelinium	3
	340	C22H28O3	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	340	C22H28O3	976-71-6	canrenone	3
	340	C22H28O3	51-98-9	Norethisterone acetate	3
	342	C21H26O4	96609-16-4	lifibrol	3
	342	C24H23NO	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	342	C22H30O3	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	342	C22H30O3	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3
	342	C23H34O2	7069-42-3	retinyl propionate	3
	342	C20H38O4	2915-57-3	bis(2-ethylhexyl) succinate	3
	342	C19H38N2O3	4292-10-8	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	3
	344	C22H32O3	520-85-4	Medroxyprogesteron	3
	344	C22H32O3	2668-66-8	medrysone	3
	344	C22H32O3	434-05-9	Metenolone acetate	3
	353	C21H39NO3	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3
	354	C20H26N4O2	3811-75-4	Hexamidine	3
	354	C22H28NO3	125-51-9	pipenzolate	3
	356	C21H40O4	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	358	C21H42O4	31566-31-1	stearic acid, monoester with glycerol	3
	360	C22H32O4	8003-24-5	4-methoxy-3-tert-butylphenol	3
	360	C22H32O4	78919-13-8	Iloprost	3
	366	C15H21Cl2FN2O3	81406-37-3	Fluroxypyr-meptyl	3
	366	C24H30O3	67392-87-4	drospirenone	3
	370	C22H42O4	103-23-1	bis(2-ethylhexyl) adipate	3
	370	C22H42O4	1330-86-5	diisooctyl adipate	3
	374	C22H30O5	1172-63-0	Jasmolin II	3
	374	C22H30O5	83-43-2	Methylprednisolone	3
	380	C17H20N2O6S	61-32-5	Methicillin	3
	388	C22H28O6	76-78-8	Quassin	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the Mjøsa sample matrices					
Matrix	RMM	Formula	CAS	Compound name	ID level
	388	C23H24N4O2		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	390	C24H38O4	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	390	C24H38O4	117-81-7	DEHP	3
	390	C24H38O4	117-84-0	Di-n-octylphthalate (DOP)	3
	392	C25H30NO3	10405-02-4	Trospium	3
	392	C24H40O4	474-25-9	chenodeoxycholic acid	3
	392	C24H40O4	128-13-2	ursodeoxycholic acid	3
	394	C23H38O5	64318-79-2	gemeprost	3
	398	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	3
	399	C18H26FN3O4S		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	400	C27H44O2	41294-56-8	alphacalcidol	3
	402	C20H34O8	77-90-7	Tributylacetylcitrate	3
	404	C23H20N2O3S	57-96-5	sulfinpyrazone	3
	410	C22H28F2O5	2557-49-5	diflorasone	3
	410	C22H28F2O5	2135-17-3	flumetasone	3
	412	C25H48O4	103-24-2	bis(2-ethylhexyl) azelate	3
	414	C24H30O6		2,6-bis(4-ethylphenyl)perhydro-1,3,5,7-tetraoxanaphth-4-ylethane-1,2-diol	3
	414	C24H30O6	107724-20-9	eplerenone	3
	418	C26H42O4	28553-12-0	Diisononyl phthalate (DINP)	3
	422	C25H42O5	1448-36-8	methyl cholate	3
	430	C27H42O4	472-11-7	ruscogenin	3
	440	C22H36N2O5S	144494-65-5	tirofiban	3
	467	C29H41NO4	52485-79-7	Buprenorphin	3
	475	C30H37NO4	126784-99-4	Ulipristal acetate	3
	501	C32H39NO4	83799-24-0	fexofenadine	3
	551	C30H53N3O6	173334-57-1	aliskiren	3
	563	C30H46NO7P	98048-97-6	Fosinopril	3
	570	C34H50O7	5697-56-3	carbenoxolone	3
	734	C40H80NO8P	63-89-8	Colfosceril-Palminat	3

Non-target screening results for LC-HR-QToF in negative ESI-mode analysis of the Mjøsa sample matrices					
Sample matrix	Molecular formula	RMM	CAS	Compound name	ID level

Zooplankton	C8HF17O3S	498,9288	1763-23-1	PFOS	3
Smelt	C8HF17O3S	498,9288	1763-23-1	PFOS	3
	C13HF25O2	662,9469	72629-94-8	PFTrDA	3
Brown Trout	C8HF17O3S	498,9288	1763-23-1	PFOS	3

Non-target screening results for GC-HRToF analysis of the rat livers

Molecular formula	RMM	CAS	Compound name	ID level
C13H10O	182,0732	119-61-9	Benzophenone	1
C12H14O4	222,0892	84-66-2	Diethyl phthalate	2
C18H36O	268,2766	7373-13-9	Methyl hexadecyl ketone	2
C16H22O4	278,1518	84-74-2	Dibutyl phthalate	2
C18H36O2	284,2715	110-36-1	Butyl myristate	2
C19H38O2	298,2872	143-91-6	Isopropyl palmitate	2
C12H5Cl5	323,8834		Pentachlorobiphenyl	2
C21H40O2	324,3028		Elaidic acid, isopropyl ester	2
C21H42O2	326,3185	112-10-7	Isopropyl stearate	2
C22H44O2	340,3341	123-95-5	Octadecanoic acid, butyl ester	2
C20H40O2	312,3028		Hexadecanoic acid	3
C21H42O2	326,3185		Methylbutyl hexadecanoate	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices

Sample matrix	RMM	Molecular formula	CAS	Compound name	ID level
Rat Liver	59,0735	C3H9N	107-10-8	propylamine	3
	71,0735	C4H9N	123-75-1	pyrrolidine	3
	89,0477	C3H7NO2	625-51-4	N-(hydroxymethyl)acetamide	3
	89,0477	C3H7NO2	107-95-9	ß-alanine	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	89,0477	C3H7NO2	107-97-1	sarcosine	3
	89,0477	C3H7NO2	56-41-7	L-alanine	3
	93,0578	C6H7N	62-53-3	Aniline	3
	93,0578	C6H7N	108-99-6	3-methylpyridine	3
	102,0681	C5H10O2	75-98-9	pivalic acid	3
	102,0681	C5H10O2	108-21-4	isopropyl acetate	3
	102,0681	C5H10O2	109-52-4	valeric acid	3
	102,0681	C5H10O2	109-60-4	propyl acetate	3
	102,0681	C5H10O2	505-65-7	1,3-dioxepane	3
	102,0681	C5H10O2	97-99-4	tetrahydrofurfuryl alcohol	3
	102,0681	C5H10O2	116-53-0	2-methylbutyric acid	3
	102,0681	C5H10O2	503-74-2	isovaleric acid	3
	103,0997	C5H13NO	3179-63-3	3-dimethylaminopropan-1-ol	3
	103,0997	C5H13NO	108-16-7	1-(dimethylamino)propan-2-ol	3
	103,0997	C5H13NO	6291-85-6	3-ethoxypropylamine	3
	104,0626	C8H8	100-42-5	Styrene	3
	110,1096	C8H14	3710-30-3	octa-1,7-diene	3
	111,0433	C4H5N3O	71-30-7	cytosine	3
	112,0273	C4H4N2O2	123-33-1	Pyridazine-3,6-diol	3
	112,0273	C4H4N2O2	1193-24-4	6-hydroxy-1H-pyrimidin-4-one	3
	115,0633	C5H9NO2	4394-85-8	N-Formylmorpholine	3
	115,0633	C5H9NO2	147-85-3	L-proline	3
	115,0633	C5H9NO2	923-02-4	N-(hydroxymethyl)methacrylamide	3
	115,0633	C5H9NO2	14205-39-1	methyl 3-aminocrotonate	3
	120,0423	C4H8O4	19757-97-2	Methyl hydroxymethoxyacetate	3
	120,0575	C8H8O	96-09-3	(epoxyethyl)benzene	3
	120,0575	C8H8O	98-86-2	acetophenone	3
	120,0939	C9H12	98-82-8	Isopropylbenzol	3
	120,0939	C9H12	95-63-6	1,2,4-trimethylbenzene	3
	120,0939	C9H12	108-67-8	mesitylene	3
	120,0939	C9H12	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	3
	120,0939	C9H12	3048-64-4	5-vinylnorborn-2-ene	3
	125,0147	C2H7NO3S	107-35-7	taurine	3
	126,0429	C5H6N2O2	4866-00-6	4-methyloxazole-5-carboxamide	3
	126,1157	C7H14N2	5351-04-2	3-diethylaminopropiononitrile	3
	128,0586	C5H8N2O2	77-71-4		3
	131,0946	C6H13NO2	61-90-5	L-leucine	3
	131,0946	C6H13NO2	622-40-2	2-morpholinoethanol	3
	134,0732	C9H10O	93-55-0	propiophenone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	134,0732	C9H10O	104-54-1	cinnamyl alcohol	3
	136,0385	C5H4N4O	315-30-0	allopurinol	3
	143,0946	C7H13NO2	7747-35-5	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	3
	143,0946	C7H13NO2	2439-35-2	2-(dimethylamino)ethyl acrylate	3
	143,9743	C2H6ClO3P	16672-87-0	Ethephon	3
	147,0718	C6H13NOS	141-98-0	O-isopropyl ethylthiocarbamate	3
	148,016	C8H4O3	85-44-9	phthalic anhydride	3
	148,0524	C9H8O2	621-82-9	cinnamic acid	3
	152,0334	C5H4N4O2	69-89-6	xanthine	3
	152,0334	C5H4N4O2	2465-59-0	oxypurinol	3
	152,095	C8H12N2O	2814-20-2	G27550	3
	158,0456	C2H11N2O4P		1,2-ethanediamine	3
	158,0844	C10H10N2	2243-62-1	1,5-naphthylenediamine	3
	158,0844	C10H10N2	479-27-6	1,8-naphthylenediamine	3
	158,1096	C12H14	4773-83-5	1,2,3-Trimethyl-1H-indene	3
	158,1096	C12H14	3748-13-8	m-bis(1-methylvinyl)benzene	3
	161,1052	C7H15NO3	541-15-1	Levocarnitin	3
	161,1056	C6H19NSi2	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	3
	162,0317	C9H6O3	93-35-6	7-hydroxycoumarine	3
	162,1409	C12H18	98-19-1	1,3-dimethyl-tert-butylbenzene	3
	162,1409	C12H18	7397-06-0		3
	162,1409	C12H18	4904-61-4	cyclododeca-1,5,9-triene	3
	162,1409	C12H18	99-62-7	1,3-diisopropylbenzene	3
	162,1409	C12H18	100-18-5	1,4-diisopropylbenzene	3
	162,1409	C12H18	25321-09-9	diisopropylbenzene	3
	164,0473	C9H8O3	156-06-9	phenylpyruvic acid	3
	164,0473	C9H8O3	15206-55-0	methyl benzoylformate	3
	164,1201	C11H16O	80-46-6	p-(1,1-dimethylpropyl)phenol	3
	164,1201	C11H16O	88-60-8	6-tert-butyl-m-cresol	3
	164,1201	C11H16O	2409-55-4	2-tert-butyl-p-cresol	3
	164,1201	C11H16O	583-03-9	fenipentol	3
	166,063	C9H10O3	120-47-8	ethyl 4-hydroxybenzoate	3
	166,063	C9H10O3	121-32-4	ethyl vanillin	3
	166,063	C9H10O3	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	3
	166,063	C9H10O3	5333-84-6	1,2,3,6-tetrahydro-3-methylphthalic anhydride	3
	166,063	C9H10O3	11070-44-3	tetrahydromethylphthalic anhydride	3
	166,063	C9H10O3	34090-76-1	tetrahydro-4-methylphthalic anhydride	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	166,063	C9H10O3	6161-65-5	2-methoxy-6-methylbenzoic acid	3
	170,0943	C9H14O3	17159-79-4	ethyl 4-oxocyclohexane-1-carboxylate	3
	170,0943	C9H14O3	1655-07-8	ethyl 2-oxocyclohexanecarboxylate	3
	180,0423	C9H8O4	50-78-2	acetylsalicyl acid	3
	182,0732	C13H10O	119-61-9	benzophenone	3
	182,0732	C13H10O	3218-36-8	p-phenylbenzaldehyde	3
	188,1565	C14H20	81-03-8		3
	188,1565	C14H20	1203-17-4	1,1,2,3,3-pentamethylindan	3
	190,1358	C13H18O	125109-85-5	ß-methyl-3-(1-methylethyl)benzenepropanal	3
	190,1358	C13H18O	103-95-7	3-p-cumenyl-2-methylpropionaldehyde	3
	190,1358	C13H18O	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	3
	193,1103	C11H15NO2	97055-05-5	metabolite CGA 37735 of S-Metolachlor	3
	193,1103	C11H15NO2	94-25-7	butamben	3
	193,1103	C11H15NO2	42542-10-9	3,4-methylenedioxymethamphetamine	3
	193,1103	C11H15NO2	1795-96-6	phenylalanine, ethyl ester	3
	193,1103	C11H15NO2	7298-73-9	N-Methylphenacetine	3
	193,1103	C11H15NO2	2631-40-5	Isoprocarb	3
	193,1103	C11H15NO2	2686-99-9	3,4,5-Trimethacarb	3
	193,1103	C11H15NO2	107447-03-0	2-Amino-1-(3,4-methylen-dioxyphenyl)-butan (BDB)	3
	193,1103	C11H15NO2	6335-76-8	ethyl 3-amino-3-phenylpropanoate	3
	194,0943	C11H14O3	94-26-8	Butyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	4247-02-3	isobutyl 4-hydroxybenzoate	3
	194,0943	C11H14O3	614-45-9	tert-butyl perbenzoate	3
	198,162	C12H22O2	88-41-5		3
	198,162	C12H22O2	111-81-9	methyl undec-10-enoate	3
	198,162	C12H22O2	688-84-6	2-ethylhexyl methacrylate	3
	198,162	C12H22O2	51000-52-3	vinyl neodecanoate	3
	198,162	C12H22O2		ethyl trans-2,2,6-trimethylcyclohexanecarboxylate	3
	198,162	C12H22O2	89-48-5	menthyl acetate	3
	198,162	C12H22O2	150-84-5	citronellyl acetate	3
	198,162	C12H22O2	713-95-1	dodecan-5-olide	3
	198,162	C12H22O2	10411-92-4	cis-4-tert-butylcyclohexyl acetate	3
	198,162	C12H22O2	20298-69-5	cis-2-tert-butylcyclohexyl acetate	3
	204,115	C13H16O2	947-19-3	Methanone, Irgacure 184	3
	204,115	C13H16O2	13893-97-5	5-methyl-1-phenylhexane-1,3-dione	3
	204,115	C13H16O2	12542-30-2	hexahydro-4,7-methano-1H-indenyl acrylate	3
	204,1514	C14H20O	80-54-6	Bucinal	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	RMM	Molecular formula	CAS	Compound name	ID level
	204,1514	C14H20O	2040-10-0	1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone	3
	206,1307	C13H18O2	15687-27-1	Ibuprofen	3
	206,1307	C13H18O2	3101-60-8	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether	3
	210,1021	C8H19O4P		Di-tert-butyl hydrogen phosphate	3
	210,1984	C14H26O		Degradation-Product	3
	210,1984	C14H26O	13019-04-0	2,4-di-tert-butylcyclohexanone	3
	218,2035	C16H26	68648-87-3		3
	220,1463	C14H20O2	719-22-2	2,6-Di-tert-butylquinone	3
	227,1885	C13H25NO2		7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole	3
	234,1256	C14H18O3	49763-96-4	stiripentol	3
	234,162	C15H22O2	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid	3
	234,162	C15H22O2	5444-75-7	2-ethylhexyl benzoate	3
	234,1984	C16H26O	54464-57-2	OTNE	3
	234,1984	C16H26O	3918-33-0	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O	16618-85-2	4-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cyclohexanone	3
	234,1984	C16H26O		Degradation-Product	3
	234,1984	C16H26O	68155-66-8		3
	234,1984	C16H26O	54464-54-9	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one	3
	234,1984	C16H26O	121158-58-5	Phenol, dodecyl-, branched	3
	241,277	C16H35N	106-20-7	2-Ethyl-N-(2-ethylhexyl)-1-hexanamine	3
	241,277	C16H35N	112-75-4	dimethyl(tetradecyl)amine	3
	241,277	C16H35N	1120-48-5	dioctylamine	3
	242,0903	C10H14N2O5	3424-98-4	Telbivudine	3
	242,0903	C10H14N2O5	50-89-5	thymidine	3
	242,2035	C18H26	1087-02-1	p-Dicyclohexylbenzene	3
	244,1787	C12H24N2O3	6425-39-4	2,2'-dimorpholinyldiethyl ether	3
	246,162	C16H22O2		Degradation-Product	3
	246,2348	C18H30	2719-62-2	6-Phenyldodecane	3
	246,2348	C18H30	25265-78-5	tetrapropylenebenzene	3
	248,1042	C6H20N2O6S	5080-22-8	N-isopropylhydroxylamine	3
	248,1049	C14H16O4	5292-53-5	diethyl (phenylmethylene)malonate	3
	248,1412	C15H20O3	71617-10-2	isopentyl p-methoxycinnamate	3
	248,1776	C16H24O2	18017-73-7	10-Phenyldecanoic acid	3
	248,1776	C16H24O2	14035-33-7	3,5-Di-tert-butyl-4-hydroxyacetophenone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	250,1933	C16H26O2		Degradation-Product	3
	250,1933	C16H26O2	2315-67-5	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol bzw 4-Octylphenol mono-ethoxylate (OPE1O)	3
	250,1933	C16H26O2	79-74-3	2,5-di-tert-pentylhydroquinone	3
	252,2089	C16H28O2	30507-70-1	(Z,E)-tetradeca-9,12-dienyl acetate	3
	253,2406	C16H31NO	68479-06-1	Propanenitrile, 3-(tridecyloxy)-, branched and linear	3
	253,2406	C16H31NO	2687-96-9	N-(n-dodecyl)pyrrolidinone	3
	258,1984	C18H26O	1222-05-5	Galaxolide	3
	258,1984	C18H26O	1506-02-1	Tonalide	3
	258,1984	C18H26O		Terphenyl, hydrogenated	3
	258,1984	C18H26O	68140-48-7	ATII (Traseolide)	3
	258,1984	C18H26O		1-(4-(trans-4-butylcyclohexyl)phenyl)ethanone	3
	260,0507	C14H12O3S	33005-95-7	tiaprofenic acid	3
	260,1776	C17H24O2		Degradation-Product	3
	262,2297	C18H30O	5892-47-7	2,4,6-tri-sec-butylphenol	3
	265,1678	C15H23NO3	6452-71-7	oxprenolol	3
	266,1552	C12H26O4S		dodecyl sulfuric acid	3
	266,1552	C12H26O4S		2-butyloctyl-sulfonic acid	3
	266,1647	C12H27O4P	126-73-8	tributyl phosphate	3
	266,1647	C12H27O4P	126-71-6	Tri-iso-butylphosphate (TIBP)	3
	266,1882	C16H26O3	19780-11-1	3-(2-dodecenyl)succinic anhydride	3
	266,1882	C16H26O3	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	3
	266,261	C18H34O		Degradation-Product	3
	268,2402	C17H32O2	21643-42-5	tetradecyl acrylate	3
	269,3083	C18H39N	112-69-6	hexadecyldimethylamine	3
	269,3083	C18H39N	124-30-1	octadecylamine	3
	272,1776	C18H24O2	50-28-2	17-beta-Estradiol	3
	272,1776	C18H24O2	57-91-0	alfatradiol	3
	276,1725	C17H24O3	456-59-7	cyclandelate	3
	276,1725	C17H24O3	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3
	276,2121	C14H32O3Si	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	3
	276,2121	C14H32O3Si	2943-75-1	triethoxyoctylsilane	3
	277,1699	C19H21N2	524-81-2	mebhydroline	3
	278,1518	C16H22O4	84-74-2	Dibutyl phthalate	3
	278,1518	C16H22O4	84-69-5	diisobutyl phthalate	3
	278,1518	C16H22O4	1962-75-0	dibutyl terephthalate	3
	278,1882	C17H26O3	3115-49-9	4-nonylphenoxy acetic acid (NPE1C)	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	278,2246	C18H30O2		2,5-bis(1,1-dimethylbutyl)hydroquinone	3
	278,2246	C18H30O2	506-26-3	gamolenic acid	3
	280,2402	C18H32O2	60-33-3	linoleic acid	3
	281,2719	C18H35NO	1593-77-7	Dodemorph	3
	282,2559	C18H34O2	112-80-1	Oleic acid	3
	282,2559	C18H34O2	2549-53-3	tetradecyl methacrylate	3
	283,2875	C18H37NO	124-26-5	stearamide	3
	284,214	C20H28O	52-76-6	lynestrenol	3
	284,2351	C17H32O3		2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate	3
	286,1933	C19H26O2	63-05-8	Androstendion	3
	286,1933	C19H26O2	846-48-0	boldenone	3
	286,2297	C20H30O	3772-55-2		3
	286,2297	C20H30O	68-26-8	retinol	3
	290,261	C20H34O	26266-77-3		3
	292,2038	C18H28O3	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	3
	292,2766	C20H36O	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	3
	294,2195	C18H30O3	2315-61-9	4-Octylphenol di-ethoxylate	3
	294,2216	C21H28N	57982-78-2	budipine	3
	297,2668	C18H35NO2	118134-30-8	Spiroxamine	3
	298,1933	C20H26O2	68-22-4	Norethisteron	3
	299,1521	C18H21NO3	125-29-1	Hydrocodone	3
	299,1521	C18H21NO3	76-57-3	codeine	3
	299,1521	C18H21NO3	968-46-7	deanol benzilate	3
	300,2664	C18H36O3	106-14-9	12-hydroxystearic acid	3
	301,2406	C20H31NO	144-11-6	trihexyphenidyl	3
	302,1882	C19H26O3	584-79-2	(RS)-3-allyl-2-methyl-4-oxocyclopent-2-enyl-(1RS,3RS;1RS,3SR)-2,2-dimethyl-3-(2-methylprop-1-enyl)-cyclopropanecarboxylate (all isomers; ratio: 1:1:1:1:1:1:1:1)	3
	302,1882	C19H26O3	560-62-3	Androst-4-ene-3,17-dione, 9-hydroxy-	3
	302,1882	C19H26O3	566-48-3	formestane	3
	302,2246	C20H30O2	58-18-4	17-alpha-Methyltestosterone	3
	302,2246	C20H30O2	153-00-4	metenolone	3
	302,2457	C17H34O4	6731-36-8	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	3
	304,2402	C20H32O2	34434-80-5	Abiet-8(14)-en-18-oic acid	3
	304,2402	C20H32O2	1424-00-6	mesterolone	3
	310,2297	C22H30O	54024-22-5	Desogestrel	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	310,2508	C19H34O3	40596-69-8	Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate	3
	312,2305	C17H36OSi2	104360-37-4		3
	314,155	C19H23ClN2	303-49-1	clomipramine	3
	314,2246	C21H30O2	13956-29-1	cannabidiol	3
	314,2246	C21H30O2	1972-08-3	delta(9)-tetrahydrocannabinol	3
	314,2246	C21H30O2	57-83-0	Progesteron	3
	314,2246	C21H30O2	1236-09-5	pregn-5-ene-3,20-dione bis(ethylene ketal)	3
	314,2457	C18H34O4	109-43-3	dibutyl sebacate	3
	314,2457	C18H34O4	110-33-8	dihexyl adipate	3
	314,2457	C18H34O4	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	3
	314,2457	C18H34O4	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	3
	314,2457	C18H34O4	871-70-5	1,18-octadecanedioic acid	3
	320,2351	C20H32O3		2-({2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]ethoxy}methyl)oxirane	3
	320,2385	C17H36O3S	111360-16-8	2-hexyldecyl mesylate	3
	327,3137	C20H41NO2	111-57-9	N-(2-hydroxyethyl)stearamide	3
	328,2402	C22H32O2	127-47-9	retinyl acetate	3
	328,2614	C19H36O4	56519-71-2	propane-1,3-diyl dioctanoate	3
	330,1831	C20H26O4	84-61-7	dicyclohexyl phthalate	3
	330,3287	C24H42	4445-07-2	octadecylbenzene	3
	333,1608	C18H24ClN3O	119168-77-3	Tebufenpyrad	3
	333,1608	C18H24ClN3O	125225-28-7	Ipconazole	3
	334,1441	C16FH19N4O3	518048-03-8	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide	3
	336,2512	C17H36O6	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	3
	337,3345	C22H43NO		docos-13-enamide, Amides, C22 (unsaturated)	3
	338,2457	C20H34O4	25155-25-3		3
	338,2457	C20H34O4	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	3
	340,1899	C19H24N4O2	100-33-4	Pentamidine	3
	340,1907	C21H26NO3	53-46-3	Methanthelinium	3
	340,2038	C22H28O3	51-98-9	Norethisterone acetate	3
	340,2038	C22H28O3	2787-02-2	17a-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	3
	340,2038	C22H28O3	976-71-6	canrenone	3
	342,1831	C21H26O4	96609-16-4	lifibrol	3
	342,1852	C24H23NO	209414-07-3	1-pentyl-3-(1-naphthoyl)indole	3
	342,2195	C22H30O3	976-70-5	3-oxopregn-4-ene-21,17a-carbolactone	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	342,2195	C22H30O3	55542-26-2	17?-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	3
	342,2559	C23H34O2	7069-42-3	retinyl propionate	3
	342,277	C20H38O4	762-12-9	bisdecanoyl peroxide	3
	342,277	C20H38O4	2915-57-3	bis(2-ethylhexyl) succinate	3
	344,2351	C22H32O3	434-05-9	Metenolone acetate	3
	344,2351	C22H32O3	520-85-4	Medroxyprogesteron	3
	344,2351	C22H32O3	2668-66-8	medrysone	3
	350,1158	C20H22O2Si2		Degradation-Product	3
	352,225	C20H32O5	363-24-6	dinoprostone	3
	352,225	C20H32O5	35121-78-9	epoprostenol	3
	353,293	C21H39NO3	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	3
	354,2056	C20H26N4O2	3811-75-4	Hexamidine	3
	354,2064	C22H28NO3	125-51-9	pipenzolate	3
	354,2076	C16H34O6S		2-(2-dodecyloxyethoxy)ethyl sulfonic acid	3
	356,1657	C18H28O5S	481-97-0	Estrone sulphate	3
	356,2927	C21H40O4	28510-23-8	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	3
	356,2927	C21H40O4	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	3
	358,3083	C21H42O4	31566-31-1	stearic acid, monoester with glycerol	3
	360,2301	C22H32O4	8003-24-5	4-methoxy-3-tert-butylphenol	3
	360,2301	C22H32O4	78919-13-8	Iloprost	3
	366,0913	C15H21Cl2FN2O3	81406-37-3	Fluroxypyr-meptyl	3
	366,2195	C24H30O3	67392-87-4	drospirenone	3
	369,3243	C22H43NO3	93-83-4	N,N-bis(2-hydroxyethyl)oleamide	3
	370,3083	C22H42O4	103-23-1	bis(2-ethylhexyl) adipate	3
	370,3083	C22H42O4	1330-86-5	diisooctyl adipate	3
	374,2093	C22H30O5	1172-63-0	Jasmolin II	3
	374,2093	C22H30O5	83-43-2	Methylprednisolone	3
	380,1042	C17H20N2O6S	61-32-5	Methicillin	3
	386,1729	C22H26O6	2618-77-1		3
	388,1886	C22H28O6	76-78-8	Quassin	3
	388,1899	C23H24N4O2		2,4-bis[N'-(4-methylphenyl)ureido]toluene	3
	390,277	C24H38O4	117-84-0	Di-n-octylphthalate (DOP)	3
	390,277	C24H38O4	117-81-7	DEHP	3
	390,277	C24H38O4	6422-86-2	bis(2-ethylhexyl) terephthalate	3
	390,277	C24H38O4	4651-67-6	3-?-hydroxy-7-oxo-5-?-cholan-24-oic acid	3
	392,222	C25H30NO3	10405-02-4	Trospium	3

Non-target screening results for LC-HR-QToF in positive ESI-mode analysis of the rat livers matrices					
Sample matrix	**RMM**	**Molecular formula**	**CAS**	**Compound name**	**ID level**
	398,2433	C18H39O7P	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	3
	399,1628	C18H26FN3O4S		(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl 5-(4-amino-5-fluoro-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolane-2-carboxylate	3
	400,3341	C27H44O2	41294-56-8	alphacalcidol	3
	402,2254	C20H34O8	77-90-7	Tributylacetylcitrate	3
	404,1195	C23H20N2O3S	57-96-5	sulfinpyrazone	3
	410,1905	C22H28F2O5	2135-17-3	flumetasone	3
	410,1905	C22H28F2O5	2557-49-5	diflorasone	3
	414,2042	C24H30O6	107724-20-9	eplerenone	3
	414,2042	C24H30O6		2,6-bis(4-ethylphenyl)perhydro-1,3,5,7-tetraoxanaphth-4-ylethane-1,2-diol	3
	415,2723	C25H37NO4	155206-00-1	Bimatoprost	3
	415,2723	C25H37NO4	89365-50-4	Salmeterol	3
	418,3083	C26H42O4	28553-12-0	Diisononyl phthalate (DINP)	3
	430,3083	C27H42O4	472-11-7	ruscogenin	3
	467,3036	C29H41NO4	52485-79-7	Buprenorphin	3
	475,2723	C30H37NO4	126784-99-4	Ulipristal acetate	3
	501,2879	C32H39NO4	83799-24-0	fexofenadine	3
	515,2917	C26H45NO7S	81-24-3	taurocholic acid	3
	532,2836	C30H41FO7	5611-51-8	Triamcinolone hexacetonide	3
	733,5622	C40H80NO8P	63-89-8	Colfosceril-Palminat	3

Non-target screening results for LC-HR-QToF in negative ESI-mode analysis of the rat livers				
Molecular formula	RMM	CAS	Compound name	ID level
C8H5F13O3S	429,9678	27619-97-2	6:2PFOS	3
C8HF17O3S	498,9288	1763-23-1	PFOS	3
C10HF21O3S	598,9279	335-77-3	PFDS	3
C12HF23O2	612,9558	307-55-1	PFDoA	3
C13HF25O2	662,9469	72629-94-8	PFTrDA	3
C14HF27O2	712,9521	376-06-7	PFTeDA	3

Norwegian Environment Agency
Telephone: +47 73 58 05 00 | Fax: +47 73 58 05 01
E-mail: post@miljodir.no
Web: www.environmentagency.no
Postal address: Postboks 5672 Sluppen, N-7485 Trondheim
Visiting address Trondheim: Brattørkaia 15, 7010 Trondheim
Visiting address Oslo: Grensesvingen 7, 0661 Oslo

The Norwegian Environment Agency is working for a clean and diverse environment. Our primary tasks are to reduce greenhouse gas emissions, manage Norwegian nature, and prevent pollution.

We are a government agency under the Ministry of Climate and Environment and have 700 employees at our two offices in Trondheim and Oslo and at the Norwegian Nature Inspectorate's more than sixty local offices.

We implement and give advice on the development of climate and environmental policy. We are professionally independent. This means that we act independently in the individual cases that we decide and when we communicate knowledge and information or give advice.

Our principal functions include collating and communicating environmental information, exercising regulatory authority, supervising and guiding regional and local government level, giving professional and technical advice, and participating in international environmental activities.