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Non-target screening – A powerful tool for selecting environmental pollutants

Preface

NILU in collaboration with UmU was engaged by The Norwegian Climate and Pollution Agency (Klif) to perform a new type of screening project which was called “non specific” or “non target” screening. The main goal with this project was to test the potential and practicalness of the available non-target screening methods for identification of unknown or new emerging environmental pollutants. It was also desired to try to estimate the quantity of the identified compounds.

Kjeller, Mars 2013

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1. Summary

This study applies the new *non-target* screening technique that means the identification of environmental pollutants without a preceding selection of the compounds of interest.

Analysis of complex mixtures in environmental samples is an extremely difficult task. Since sample matrices in most cases are complex, traditionally ultra trace analytical methods were specifically developed for a certain type of sample and group of substances. This traditional *targeted* approach gives good sensitivity and reliable identification and quantification of the target compounds, and has been used with success for several decades. However, this traditional approach has a significant drawback as it always will miss all compounds which were not selected at the start of the analyses, that means normally all unknowns or other untargeted substances even in high concentrations or with severe toxic potential. There are good reasons to believe that the concentration of the unknowns or unidentified compounds exceeds by fare the concentration of the known's. In addition effect studies have shown in many cases that the concentrations of the known compounds are not high enough to explain some of the toxic potentials of samples. To fill this knowledge gap *non-target* screening methods are very important tools for environmental chemistry. During the last decade new analytical hardware and software tools have been developed which make a non-target screening approach much more realistic and affordable today than in earlier years.

To get a better impression of the strength and weaknesses of this method and in order to establish an operative method in Norway, Klif initiated this small pilot study which includes a broad selection of different samples which are most relevant in environmental research and monitoring. Due to limitation in time and budget it was not possible to have a dedicated field campaign and to select sampling sites in a systematic and logical manner. It was therefore decided to use samples which were already at NILUs laboratory due to other projects. The following sample types were chosen for this initial test: ambient air, sewage water and sludge, sediment, and different types of biota. All the samples were prepared in duplicate and analyzed by different state of the art techniques for non-target screening analysis. The raw data from instrumental analysis were treated with newly developed and very advanced software tools tailored to filter out as most as possible of relevant information.

The main goal of this project was achieved without any deduction, namely to proof that non-target screening is a practical and useful tool for identification of unknown or new emerging environmental pollutants. It was possible to identify huge number of new or earlier unrecognized contaminants in different environmental samples. The following compound classes were identified and partially quantified in this study: pharmaceuticals and personal care products (PPCP) including perfumes and biocides, polycyclic aromatic compounds (PACs), polymer additives and other compounds used in technical applications including phthalates/adipates, antioxidants, benzothiazoles/triazoles, and branched alkylated benzenes (BABs), pesticides, and halogenated compounds (prevailing chlorinated and brominated compounds).

It was also asked if it is possible to estimate the quantity of the identified compounds in an easy and straightforward way. This is unfortunately only possible for compounds detected by the GC-MS methods. The reason for that is the tremendous variation of ionization potential and hence response in the available LC-MS methods. The only way out of this is to calibrate the LC-MS system with an isolated standard of the compound of interest. That means quantification is in principal possible for all detected compounds, however, in some cases this may be quite complicated, work intensive, and thus also expensive. On the other hand the use of isolated standards is also the most reliable way to finally proof and verify the tentatively identification, and is one of our most important recommendations:
We recommend to verify, compare and discuss the list of tentatively identified compounds against isolated standards and what is known about use, environmental occurrence, and environmental and toxic effects.

In order to use the full potential of the ToF-MS technique for non-target screening and especially retrospective analysis at a later stage, we strongly recommend to include this analytical technique in future screening and more regular monitoring studies.

Before starting more work on risk assessment and potentially regulatory measures we strongly suggest to start the verification of these initial findings by more sophisticated studies. This should include a dedicated sampling strategy either to proof atmospheric long range potential and persistency, or bioaccumulation potential.

To take the full advantage of the data and knowledge generated during this study and to stimulate the national and international research in this field we suggest to report the verified data into the databases of the European network of laboratories monitoring emerging pollutants (NORMAN).

2. Sammendrag

Denne studien anvender en ny "non-target" eller "ikke spesifikk" screening metoden. Det vil si at man prøver å identifisere miljøgifter uten at man allerede på forhånd velger hvilken stoffer man vil se på.

Det å utføre kjemisk analyse av komplekse stoffblandinger man finner i miljøprøver er en veldig vanskelig oppgave. Prøvematriksen i slike prøver er ofte veldig sammensatt og i tradisjonell ultrasporanalyse bruker man ofte analysemetoder som er spesialtilpasset både prøvetype og analysert substansgruppe. Denne tradisjonelle målrettete (*target*) tilnærming gir som regel en god analytisk følsomhet, pålitelig identifikasjon og kvantifisering av de utvalgte komponenter (analytter). Denne metoden har med hell vært brukt i flere tiår. Den største ulempen med denne tradisjonelle metoden er at man ikke ser stoffer som ikke er blitt valgt ved starten av analysen. Det betyr at man mister alle ukjente forbindelser og alle stoffer som er valgt bort ved starten, selv om det kan være tilstede i høye konsentrasjoner eller utgjøre et betydelig toksisk potensial. Det er mye som tyder på at det i mange prøver finns en høyere konsentrasjon og et større antall ukjente enn kjente forbindelser og ofte er det toksiske potensialet som måles i miljøprøver større enn det som kan forklares gjennom de påviste og kvantifiserte stoffer. En viktig metode for å identifisere disse ukjente forbindelser i miljøprøver er en screening metode som betegnes som *non-target* screening. Den siste tids utvikling av nye analyseinstrumenter og programvare gjør at en slik *non-target* screening er mer realistisk og overkommelig enn for bare noen få år siden.

For å få en bedre oversikt og inntrykk av styrker og svakheter av denne metoden ble det igangsatt et lite pilotprosjekt av Klif. Prosjektet omfatter de fleste typer av miljøprøver som kan være relevante i forskning og overvåkning av miljøet. Både tid og budsjettbegrensninger tillot ingen dedikert og systematisk prøvekampanje og prosjektet begrenset seg til prøver som gjennom andre prosjekter var tilgjengelig ved NILUs laboratorium i den aktuelle perioden. Prøvene ble ekstrahert og analysert med forskjellige "state-of-the-art" analyseteknikker som er tilgjengelig for denne typen non-target screening analyser. Den største utfordringen og det meste av tidsforbruket var knyttet til å få etablert og gjennomført filtrering og tilrettelegging av det ekstremt store rådatasettet.

Hovedmålet i prosjektet ble oppnådd uten reservasjon: non-target screening er en metode som er praktisk gjennomførbar og et veldig nyttig verktøy for identifikasjon av ukjente stoffer og nye miljøgifter. I denne studien var det mulig å påvise et stort antall nye eller tidligere ikke identifiserte stoffer i de forskjellige studerte typer miljøprøver. Stoffer i følgende stoffgrupper ble identifisert og delvis også kvantifisert: stoffer i legemidler og kosmetikk (PPCPs) inklusive parfymestoffer og biocider, polysykliske aromatiske komponenter (PACs), additiver til polymerer/tekniske komponenter (ftalater/adipater, antioxidanter, benzotiasoler/triazoler og forgrenete alkylerte benzener), pesticider, og forskjellige klor- og bromorganiske forbindelser.

Det var også ønskelig å prøve å gjennomføre en bestemmelse eller i det minste estimere konsentrasjonen av de identifiserte stoffene på en enkel måte. Dette er dessverre bare mulig for de av stoffene som ble målt ved hjelp av GC-MS teknologien. Grunnen til det er at med LC-MS som er den alternative metoden, så varierer ioniseringspotensial og dermed instrumentets følsomhet alt for mye og ofte med mange størrelsesordener. Eneste utvei er å kalibrere instrumentet med en kjent mengde av de respektive stoffene. I mange tilfeller er dette mulig, men en tidkrevende og relativ kostbar oppgave. I andre tilfeller er stoffene ikke tilgjengelig som isolert standardmateriale slik at det ikke er sikkert at det lar seg gjennomføre. På den andre siden er en slik kalibrering av instrumentet også det som må til for en entydig identifisering av den tentative identifikasjonen av stoffene og er en av de viktigste anbefalinger for oppfølging av denne studien:

Vi anbefaler å bekrefte forekomst av disse stoffer ved injeksjon av isolerte standardforbindelser og sammenligne og diskutere stoffenes forekomst med dagens kunnskap om bruk, forekomst i miljø og effekter på miljø og helse.

Resultatene fra denne studien må bekreftes gjennom mer dedikerte studier før de kan brukes i risikovurderinger eller som grunnlag for reguleringer. Dette vil innebære dedikerte prøvetakingsstrategier for å fastslå langtransport- og bioakkumuleringspotensial samt persistens i miljøet.

Videre bør potensialet av ToF-MS teknologien utnyttes mer for både denne typen non-target screening studier og spesiell for retrospektive analyser ved å kjøre en del av de planlagte target målingene ved ToF-teknikk og en rådatafiltrering ved et senere tidspunkt.

For å kunne utnytte fordelen med denne metoden fullt ut og for å stimulere og støtte den internasjonale forskning på dette feltet anbefales det at de verifiserte data og massespektra legges inn i databasene fra det europeiske nettverket (NORMAN) som jobber i det feltet.

Non-target screening – A powerful tool for selecting environmental pollutants

3. Introduction

This study applies the new *non-target* screening technique that means the identification of environmental pollutants without a preceding selection of the compounds of interest.

Analysis of complex mixtures in environmental samples is an extremely difficult task. Since sample matrices in most cases are complex, traditionally ultra trace analytical methods were specifically developed for a certain group of substances. This traditional *targeted* approach gives good sensitivity and reliable identification and quantification of the target compounds, and has been used with success for several decades (Arp et al., 2012). However, this traditional approach has a significant drawback as it always will miss all compounds which were not selected at the start of the analyses, that means normally all unknowns or other untargeted substances even in high concentrations or with severe toxic potential. There are good reasons to believe that the concentration of the unknowns or unidentified compounds exceeds by fare the concentration of the known's. In addition effect studies have shown in many cases that the concentrations of the known compounds are not high enough to explain some of the toxic potentials of samples. To fill this knowledge gap *non-target* screening methods are a very important tool for environmental chemistry.

During the last decade mass spectrometer (MS) based on time-of-flight technology (TOF-MS) has become more affordable, stable, and useful for environmental trace analysis. TOF-MS acquire full mass spectra with a much better sensitivity than a standard quadrupole MS and make it a versatile tool for both target and non-target analysis of environmental contaminants. Combined with gas or liquid chromatography (GC-MS or LC-MS) it is possible to separate and detect a very broad range of chemical compounds (Figure 1) in only one or a few single runs.

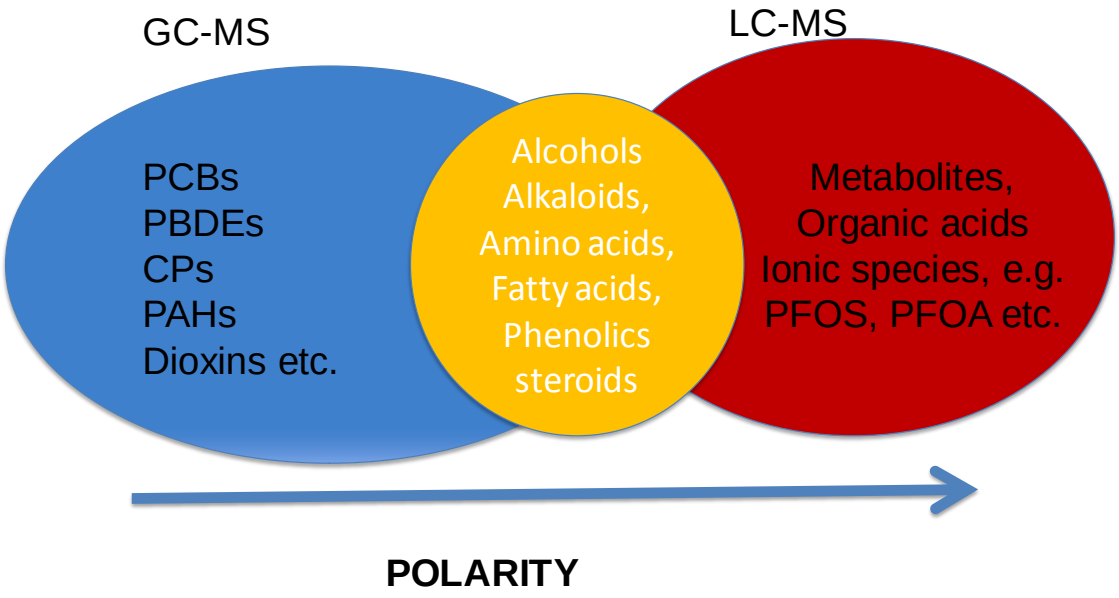

Figure 1: Typical application range for GC-MS and LC-MS

An important new feature of ToF-MS is the possibility to examine old full scan data files in a retrospective way in order to look for environmental contaminants which earlier were unknown, overseen or of minor interest. Unfortunately, this feature is not fully recognized and valued yet, but future screening and monitoring studies will take substantial advantages of this possibility.

Another important technical development of the last years is comprehensive two dimensional GC. This technique can separate coeluting compounds and gives a superior separation power and also a better sensitivity than single GC-techniques. This feature is illustrated in Figure 2 (upper left drawing), where the compounds A and B are not separated in the normal 1-dimensional GC separation (often described as coeluting compounds). However, when using a different chromatographic phase in the second dimension it might be possible to separate compound A and B (Figure 2, lower left drawing).

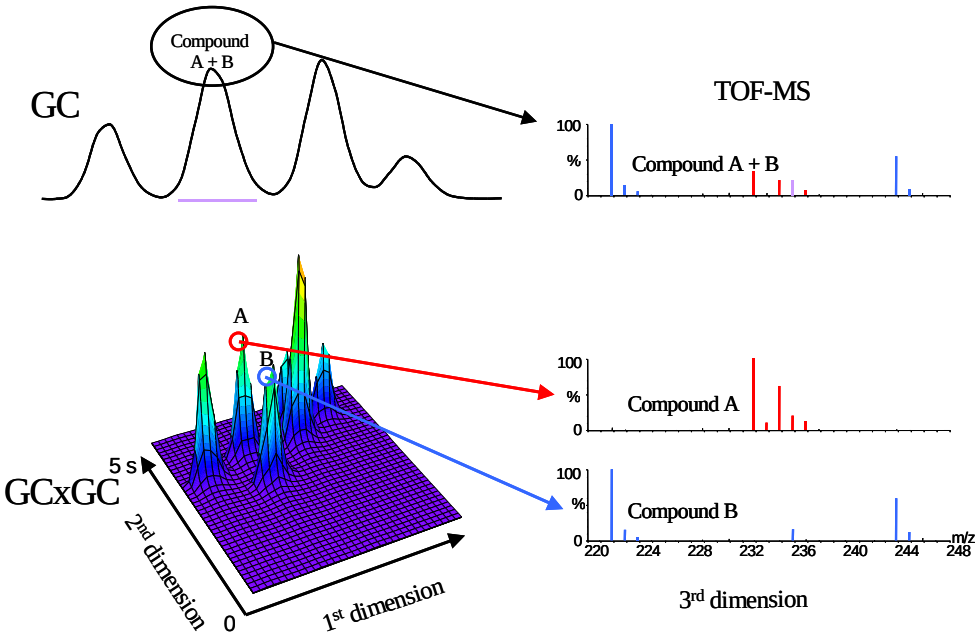

Figure 2: 1-dimensional and 2-dimensional GC combined with ToF-MS (GC-MS and GCxGC-MS

The study presented in this report applied state of the art techniques, namely GCxGC-LRToFMS, GC-HRToFMS, and LC-HRToFMS, to a limited selection of samples often used for environmental contamination studies. For the necessary data-mining the raw data from instrumental analysis were treated with newly developed and very advanced software tools tailored to filter out as most as possible of relevant information.

4. Theoretical background

4.1 Principles of compound identification by mass spectrometry

A chemical substance is unequivocally described by its systematic names (often IUPAC name), different types of identifiers registry numbers (CAS entry number or other numbers), or its structural formula (Figure 3).

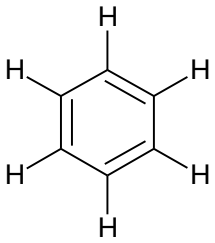

Figure 3: Structural formula of benzene (IUPAC name), cyclohexa-1,3,5-triene (systematic name), or 71-43-2 (CAS entry number).

The most commonly used method for analysis or compound identification in the field of environmental contaminants is based on mass spectrometry. With mass spectrometry using a soft ionization technique (normal situation in LC-MS) we get in many cases the mass of the ionized molecule. When using high enough mass resolution (accuracy of the mass determination) which is available at the more advanced ToF-based mass spectrometers, we can normally calculate one or several molecular or chemical formula. In the case of benzene this molecular formula is C_6H_6 which tells us the number of different atoms that constitutes a particular chemical compound. However, this type of description is only an unequivocal identification for the simplest molecules. For C_6H_6 we have already 217 different structural possibilities or different isomers (Figure 4).

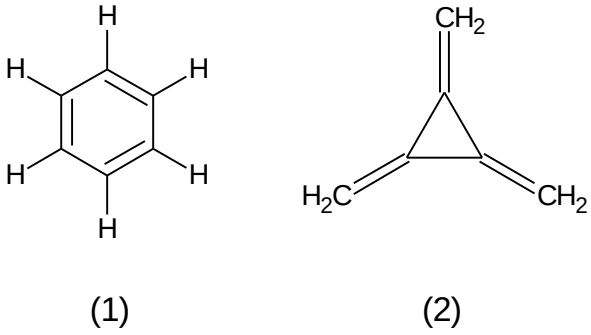

Figure 4: Structural formula of 2 of 217 possible structures for C_6H_6: (1): Benzene, (2): 1,2,3-tris(methylene)-cyclopropane,.

That means that we need more information to elucidate the exact structure of the measured compound. Either by using a higher ionization energy by electron impact ionization (normally used in GC-MS) or by inducing collision of the molecules it is possible to induce fragmentation of the molecular ion into different fragments, see Figure 5. The distinct patter of the fragments can be used to read out structural information either by a theoretical interpretation of the mass spectrum or most often by comparing it with spectral libraries. In many cases this allows a tentatively identification of the substance or at least the class of substance.

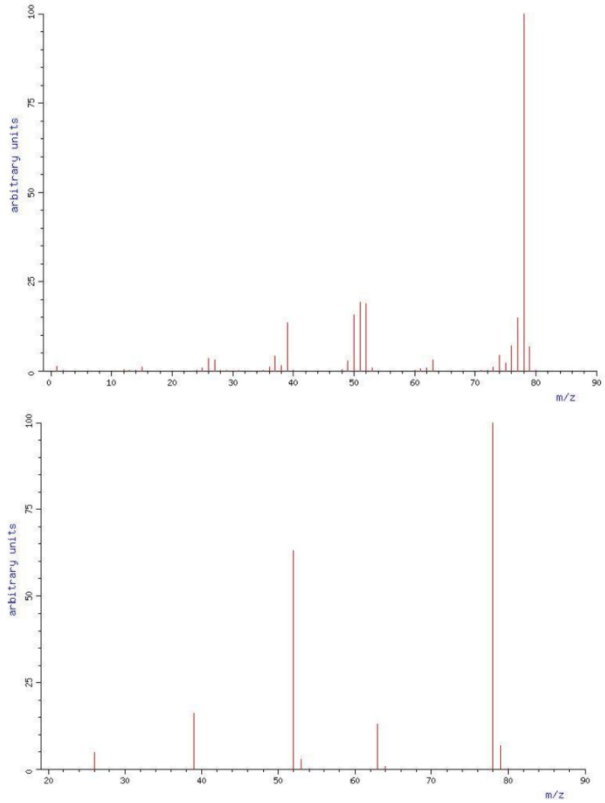

Figure 5: Mass spectrum of (1): Benzene and (2): 1,2,3-tris(methylene)-cyclopropane.

4.2 Use of chromatographic methods for separation and structural information

By applying either gas or liquid chromatographic methods before introducing the analytes (compounds of interest) into mass spectrometer (GC-MS or LC-MS) we achieve a separation of the mass spectral signals which make the MS-information easier to understand and evaluate. However, we can also use the retention time of each analyte to get an idea about their boiling point/volatility (GC) and polarity (GCxGC and LC), see Figure 6 (Muusse et al., 2012). These parameters can be used for a further reduction of the possible structures/compounds.

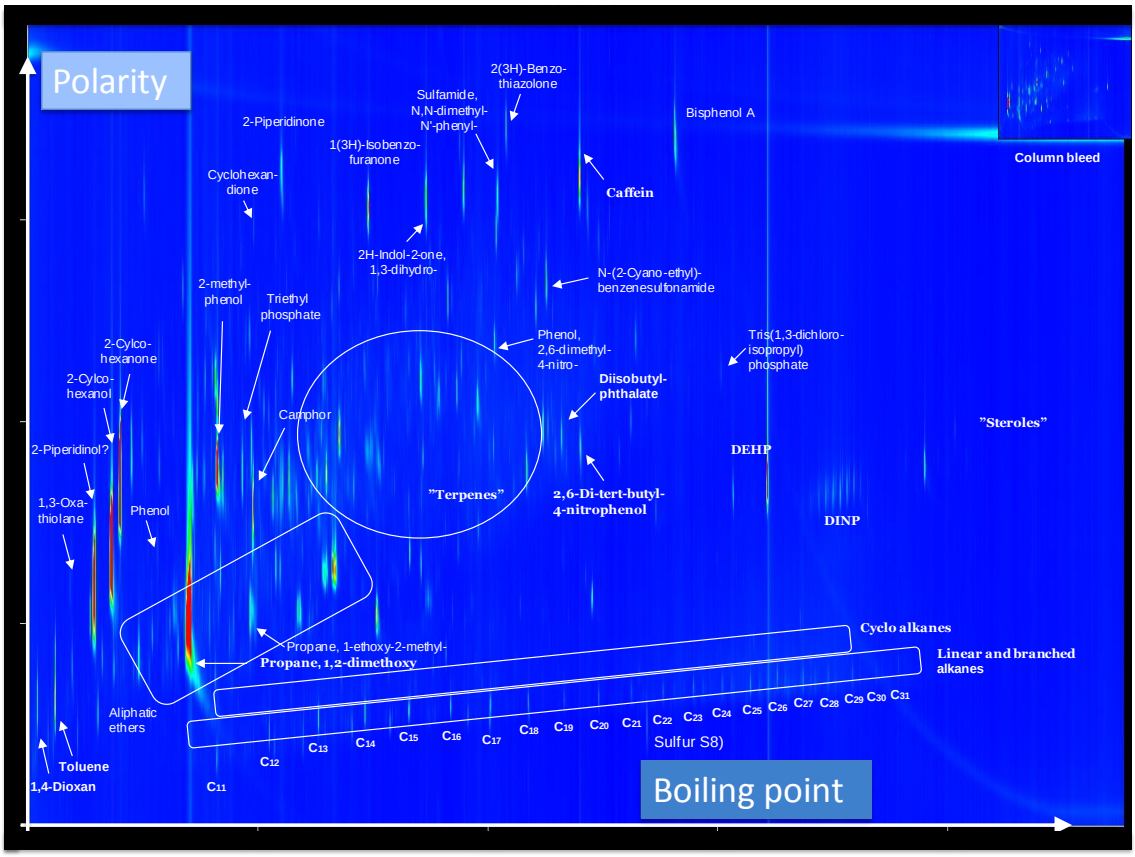

Figure 6: GCxGC chromatogram of a waste water sample illustrating compound separation according to boiling point/volatility in the first dimension and polarity in the second dimension.

The principles of compound identification outlined in the chapter above were originally developed for single and isolated compounds. Chromatographic separation units as GC or LC mounted and applied up-front the MS-detection allow either a complete or at least a partly separation of complex mixtures which are normally found in environmental sample extracts. Whereas traditional 1-dimensional GC have the capacity to separate up to 100s of different compounds, comprehensive 2-dimensional GCxGC technique can separate more than 1000s of compounds in one single 30 min run. Mass spectrometry which separates compounds by their mass, add an additional dimension of separation. However, in order to sort out the different mass spectra of the different compounds, we can take considerable advantage of a modern mathematical algorithm, namely deconvolution. With deconvolution algorithms we can even separate peaks which are coeluting (Figure 7). The applied software tools and databases are described in more detail in chapter 5.3.3 and 5.4.3 (Bastos and Haglund, 2012, Muusse et al., 2012, Rostkowski et al., 2011)

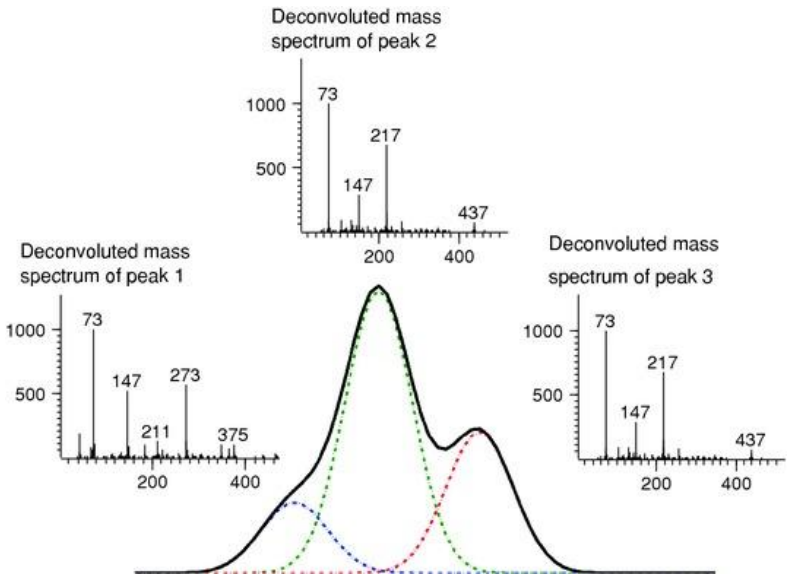

Figure 7: Illustration of the results of chromatographic peak deconvolution.

4.3 Limitations

For this non-target screening study we have chosen very general approach using the newest and most advanced analytical instruments available at the time which allow us to potentially detect as many as possible different compounds. However, there are some methodical limitations which mean that the following compound classes may not be detected:

1. Compounds not dissolved in the solvents selected for this study, acetonitril/methanol or dichloromethane. Typical compound groups are dyes and pigments, salts, and metals.
2. Nonvolatile and/or labile compounds will not pass through the GC separation and will thus not be detected by the GC-MS methods (but in many cases by LC-MS). This may be due for some of the highest brominated flame retardants.
3. In LC-MS it is normally possible to get all compounds through the LC separation. However, a characteristic of LC-MS is that the response or detection sensitivity can be very different from one compound group to another. Whereas some compound groups can have exceptional high sensitivity other groups may only have limited or no sensitivity at all. The reason for this compound property can be explained by the different potential for ionization. This feature explains also why it is not possible to estimate a concentration of compounds detected and identified. The typical application range of GC-MS and LC-MS is shown in Figure 1.
4. In general compounds of low concentration might be masked by compounds of very high concentration eluting with the same retention time and nearby masses.
5. Distinction between natural and anthropogenic compounds is not straightforward, and is mainly based on the information given in the applied databases.

5. Methods

5.1 Sampling

As this study was designed as a pilot study with the intention of testing the possibilities, strengths, weaknesses of the non-target screening approach, it was necessary to select very broad selection of different samples which are most relevant in environmental research and monitoring. Due to limitation in time and budget it was not possible to have a dedicated field campaign and to select sampling sites in a systematic and logical manner. It was therefore decided to use samples which were already at NILUs laboratory by coincidence or which were easily sampled without a lot of extra expenses. The following sample types were chosen for this initial test: ambient air, sewage water and sludge, sediment, and different types of biota (see Table 1).

Table 1: Information on samples selected for this study.

Sample type	Comments	Sample amount
Air (remote)	Birkenes filter	339 m3
Air (urban)	NILU filter	54 m3
STP	Digested sludge	5 g
STP	Raw sludge	5 g
STP	Influent	75 mL
STP	Influent particles	75 mL
STP	Effluent	750 mL
Sediment	Frierfjorden	5 g
Biota	Prawns- Eidanger	2.5 g
Biota	Cod liver- Sørfjorden	2.5 g
Biota	Egg Common eider - Runde	2.5 g
Biota	Egg Common shag - Runde	2.5 g
Biota	Egg Herring gull - Runde	2.5 g

This approach is satisfactory to illustrate and proof the possibilities of the non-target screening approach. However, this test approach restrict considerable the possibilities for further discussions and conclusions on spatial distribution, bioaccumulation, and long range transport potential.

5.2 Sample extraction

All the samples were prepared in duplicate, one to be extracted for LC-TOF analyses and another for GCxGC and GC-HR-TOF analyses.

5.2.1 Wastewater influent/effluent and influent particle

Wastewater influent and effluent samples (75 and 750ml, respectively) were extracted with Waters Oasis SPE cartridge in parallel with dichloromethane as an elution solvent of the samples used in GCxGC-TOF and GC-HR-TOF analyzed and with methanol/acetonitrile (50:50) for the purpose of LC-HR-TOF analyses. In order to avoid clogging the SPE cartridges with particles influent samples were passed through a glass fiber filter prior to extraction. All filters containing particles were extracted in the ultrasonic bath with solvents chosen for different analytical techniques.

5.2.2 Sediment and sludge

Sediment and sludge samples prior to extraction were mixed with activated copper powder to remove elemental sulphur and then approximately 5 g was extracted using ultrasonic bath with dichloromethane (for gas chromatography mass spectrometry analyses) and with acetonitrile:methanol for LCMS analyses.

5.2.3 Biota samples

In order to remove water samples were treated with anhydrous sodium sulphate and extracted in the ultrasonic baths with either dichloromethane or methanol:acetonitrile (50:50)

5.3 GCxGC-MS and GC-HRMS methods

5.3.1 Sample pretreatment

The samples with heavy matrix, i.e. sludge, sediment and biota samples, were subjected to filtration, dichloromethane extraction and non-discriminating gel permeation chromatography (GPC) clean-up. Sediment and sludge samples were also treated with cupper powder to remove elemental sulfur. All samples were then concentrated to ca 100µL and analyzed by both techniques. The total ion chromatograms revealed a relatively high “background” of lipids in several “heavy matrix” samples and these samples were therefore filtered through silica using acetone:hexane (1.1, v/v), and were reanalyzed.

5.3.2 Instrumental analysis methods

The GCxGC-MS analyses were performed using a Leco 4D equipped with a HP6890 GC and a 30m x 0.25mm x 0.25µm SGE BPX-50 (50% phenyl-methylsilicone) and a 2m x 0.15mm x 0.15µm Varian VF-1ms (100% methylsilicone) column. Helium was used as carrier gas at a constant flow of 1 ml/min and the GCxGC modulator was operated at a modulation frequency of 7s. The main GC oven temperature program was 60°C (1 min) – 5 C°/min – 300°C (2 min) and the second oven was ramped at +20°C bias. One microliter aliquots was injected in the split-less mode and EI mass spectra (70 eV) was collected at 100 Hz over the mass range 35-700 Dalton.

The GC-HRMS analyses were performed using a Leco GC-HRT equipped with a HP7890 GC and a 30m x 0.25mm x 0.25µm J&W DB5MS-UI (5% phenyl-methylsilicone). Helium was used as carrier gas at a constant flow of 1 ml/min. The GC oven temperature program was 60°C (1 min) – 5 C°/min – 300°C (2 min). One microliter aliquots was injected in the split-less mode and EI mass spectra (70 eV) was collected in the high-resolution mode (>25000 resolution) over the mass range 35-700 Dalton.

5.3.3 Data treatment

The automatic GCxGC peak detection and deconvolution routine was used with a signal-to-noise ratio of 20 and the spectra was compared to the NIST 2011 library. Peaks with "similarity" >700 (70% match) was manually evaluated. Candidates that did not hold for this inspection were discharged. Similarly, peaks that also were detected in the blanks were eliminated. The remaining components were semi-quantified vs. the internal standard (D10-phenanthrene) using MS Excel and were annotated. CAS number was presented for components with "unambiguous" spectra. For the remaining, a chemical class was assigned.
The GC-HRT data was very complex and it as clear that the chromatographic resolution was not sufficient for this type of complex matrices. Consequently, the automatic peak detection and deconvolution routine produced fewer tentative structures than GCxGC-MS and mostly for high abundance components. It was however useful for confirmation/discrimination of GCxGC candidates. In addition, the isotope filter option of the software proved useful to automatically detect halogenated (chlorinated and brominated) compounds in the samples.

5.4 LC-MS analyses

5.4.1 Sample pretreatment

5.4.2 Instrumental analysis methods

LC-HR-TOF analyses were performed with Agilent 1290 Infinity UHPLC coupled with Agilent 6530 QTOFMS with Agilent JetStream ESI source operated in positive and negative modes. Samples were separated using a reverse phase Waters Acquity UPLC HSS T3 column (100Å, 1.8µm, 2.1 mm x 100mm). Mobile phases A and B were water with 0.1% formic acid, acetonitrile with 0.1% formic acid (positive mode) and water with 0.1% ammonium acetate and methanol with 0.1% ammonium acetate (negative mode). Separation was achieved using a flow rate of 0.4 ml/min with the following gradient: 90:10 to 78:22 in 3.5 min, 50:50 at 20min and 0:100 at 30min for 10 min.

5.4.3 Data treatment

Raw LC/MS data was analyzed with Agilent Mass Hunter Qual software. In the first step molecular feature extraction module (MFE) was used to find peaks in the total ion chromatogram. The software removed the chemical background from the three dimensional LC/MS dataset, found the true ion signals, grouped the chemically related ion signals (isotopes, adducts and dimmers). This resulted in a compound table with associated chromatograms and pure spectra with each compound with a quality score calculated. As a compromise, to avoid extracting too much of background noise only peaks with more than 50-500 counts (sample dependent) and quality score over 60% were extracted. To take advantage of mass accuracy of the data the results of this data processing were further used to derive molecular formulas of compounds extracted by the MFE feature. Besides accurate mass additional mass spectral information (isotope ratios and isotope mass values) were used to logically narrow the list of possible formulas. Following elements were selected as acceptable in this procedure: C,H,O,N,S,Cl,Br, P with a minimum overall score per charge carrier set to 35 and a mass error window defined to 5ppm. For each compound, a probability score was calculated that is based on how well the isotope abundance ratios for the candidate molecular formulas match those from the experimental data. This resulted in a shorter list of ranked candidate molecular formulas, with the top score (highest score = 100) being more likely to be correct. In the last step the formulas with overall score of 80 % and up were compared with Agilent databases of contaminants and a public database Chemspider. It allowed for a tentative identification (based on the possibility of the compound to be likely present in the tested sample) of some structures and for a provision of elemental formulas of compounds with too many candidates in these libraries.

Overall relative score was calculated based on scores from different steps in the structure elucidation procedure with the assumption that lack of the candidate or too many candidates in databases were not decreasing overall score of compounds with only elemental composition available.
Based on this approach a number of environmental contaminants have been tentatively identified with lists of compounds or molecular formulas with overall score of minimum 60 % presented. This allowed filtering out lower quality data, for example to delete initially interesting formulas containing 2 or more chlorine atoms but with missing isotope pattern in the spectra. However it is important stress out this approach could sometimes cause deletion of compounds with low concentration or a partial removal of isotopes, which would cause lowering the overall score of compounds likely present in the sample and therefore their removal from the list of identified compounds.

More research is recommended to confirm the identities of interesting emerging compounds and this include analyses of pure standards whenever possible, MS/MS experiments and predictions of retention time, when the standard is not available.

6. Results and Discussion

6.1 General overview of results

The quality of the information generated by this study were very variable. In worst cases we had only some analytical signals without any extra information in databases, and in best cases it might even be possible to perform an unequivocal identification of the compound together with an exact quantification of the compound concentration. Roughly the results can be grouped into 5 different quality classes:

1. Unknowns with known retention times and mass spectra (not listed),
2. Unknowns with known retention times, mass spectra, and molecular formula (listed as unidentified in Appendix),
3. Unknowns with known retention times, mass spectra, molecular formula, and some structural information (listed as unidentified in Appendix),
4. Tentatively identified compounds (listed with compound name and CAS number in Appendix),
5. Identified and verified compounds (not available in this study).

In the frame work of this project, only results of class 1 to 4 were generated. In order to lift up results from class 4 to 5 it is necessary to prepare standard solutions of the tentatively identified compounds and inject it into the system at the same settings as for the sample. Due to time and partly also economical restrictions that was not possible.

In the appendix two different sets of results (GC-MS and LC-MS) with a quality class 2 to 4 are listed for each of the measured samples. For each sample two table are shown, one for the GC-MS and one for the LC-MS runs.

The tables are built up by compound name, CAS entry number, molecular formula, similarity/score, compound class, and a comment field. For the compounds determined by GC/MS-technique an estimated amount is given in this table in ng/sample. Dividing this number by sample amount listed in Table 1 it is possible to calculate the concentration. However, these results are semi-quantitative estimates and should be treated and discussed with extreme caution.

The number of detected compounds is summarized as detection frequency in Table 2. It is important to note that identification frequencies in Table 2 are only valid for the similarity- or score-factor used at this time. Slight variations in sample amount, instrument sensitivity or score-factor settings would change the figures dramatically.

Table 2: Number of detected compounds for some important compound groups for the analyzed samples. The identification frequency is illustrated by a colour code from green = low via yellow = medium to red = high detection frequency.

Sample type / Compound group	Air		STP					Sediment	Biota					Sum
	Remote	Urban	Digested sludge	Raw sludge	Influent	Influent particles	Effluent	Contaminated fjord	Prawns	Cod liver	Common eider	Common shag	Herring gull	
Unidentified	252	212	265	82	271	291	209	237	305	63	216	230	286	2919
PPCPs	26	18	39	25	33	15	242	25	39	54	33	4	34	587
PACs	1	9	50	94	9	3	4	96	45	0	4	2	2	319
Additives	12	15	27	42	34	15	28	15	9	6	8	3	5	219
Phthalates	9	8	8	8	7	8	8	17	1	1	0	0	1	76
Organophosphates	4	7	4	7	7	4	9	5	3	2	2	4	7	65
Pesticides	4	5	5	4	2	2	33	1	5	1	6	2	12	82
Halogens	0	0	6	6	0	1	0	12	0	14	2	10	29	80
Oxy-compounds	0	0	0	12	9	0	4	7	0	0	0	0	0	32
N-compounds	0	0	2	7	1	0	2	0	0	0	0	0	0	12
PFCs	0	0	0	0	3	0	0	0	1	0	0	0	0	4
Sum identified	56	62	141	205	105	48	330	178	103	78	55	25	90	1476
Sum	308	274	406	287	376	339	539	415	408	141	271	255	376	4395

PPCPs: Pharmaceuticals and personal care products,
PACs: Polycyclic aromatic compounds,
Additives: Polymer additives and different other compounds used in technical applications,
Halogens, oxy-, and N-compounds: Compounds not registered in the above groups containing halogen, oxygen, or nitrogen atoms in the organic molecule.

6.2 Identified compounds of special interest

Not very surprising the number of unidentified compounds is far higher than the number of even tentatively identified compounds. However, many of these unidentified compounds may be natural compounds and thus of minor interest for this study. Beside a considerable number of already known compounds, there were also quite a number of compounds which either were not detected in these types of samples or only reported occasionally. It must be mentioned that the selection of compounds which will be discussed further in this chapter, is rather subjective and not based on a strong scientific justification.

6.2.1 PPCP

The compounds of the group of pharmaceuticals and personal care products (PPCP) were found in all samples analyzed in this study. Even when recognizing some problems with possible false positives as mentioned in chapter 6.3.4, there are many compounds which need to be studied by a more specific and targeted approach.

Very prominent in sewage samples are the compound class of fragrances/perfumes with compounds like Tonalide, Galaxolide, Cedrene, Kaurene, Cedrol, Ionone, and several other compounds. The estimated concentrations are in the range of 1 to 100 ng/g d.w. (digested sludge) or 1 – 10 ng/L (effluent).

Benzophenone which is used in both cosmetics and technical products as an UV-filter is not only found in contaminated sediment and sewage samples (~ 1 - 100 ng/g d.w.) but also in the remote air sample (~ 10 pg/m^3).

Pharmaceuticals were mainly detected by LC-MS techniques and the list of tentatively identified compounds is for some of the samples extremely long. Due to the variability of instrument response (see chapter 4.3) the compound concentration could not be estimated and thus the relevance of the results and prioritization for follow-up is very difficult. As the next step for follow up we would suggest to focus on verification and quantification of the already existing data, before new field campaigns are started.

6.2.2 PACs

The group of polycyclic aromatic compounds (PACs) with the group of polycyclic hydrocarbons (PAHs) as a subgroup is found in nearly all samples and sometimes with a lot of different compounds and with quite high concentrations. Many members of this group are already known as strong carcinogenic compounds, therefore it would be wise to cross check the lists generated in this study with the available information on toxicity.

Most of the compounds are often described as unintentionally produced contaminants. However, this classification is not valid for some of the PACs, as for example the different Diisopropylnaphthalenes found quite frequently in this study (air ~ 20 pg/m^3; sewage/sediment ~ 1 - 5 ng/g; ~ 5 - 30 ng/L). These compounds are marketed as a high boiling solvent for both epoxy and PUF production and for carbon less copy papers.

6.2.3 Additives

Under this heading polymer additives and different other compounds used in technical applications are listed, however, phthalates and organophosphates are listed separately. One compound found in all abiotic samples in high concentrations is Oleyl nitrile (112-91-4). However, since this compound is used in nitrile rubber a contamination of these samples during sampling/clean-up/storage cannot be excluded completely, and the results should therefore be treated with some caution.

Antioxidants

Different antioxidants of the phenolic type (BHT and related compounds) were found in nearly all samples even in one biota sample (air ~1 – 10 ng/m^3; sewage/sediment ~ 1 - 100 ng/g; ~10 ng/L; egg: ~100 ng/g f.w.). Some of these compounds were detected in earlier studies, however, some are found for the first time in Nordic samples: 2,6-bis(1,1-dimethylethyl)-1,4-benzenediol (CAS: 2444-28-2) and its oxidized form 2,6-bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione (CAS: 719-22-2) were found in high concentrations in the contaminated sediment sample (Frierfjord) ~100 ng/g d.w..

Benzothiazoles and benzotriazoles

Two different groups of heterocycles, namely the benzothiazoles and the benzotriazoles, were found in many different samples (Benzothiazole: air: ~100 pg/m^3; sewage sludge: ~ 1 – 5 ng/g; sewage influent: ~1,5 µg/L effluent: 4 ng/L) . Some but not all of this compounds were earlier found in screening studies. One derivative, 2(3H)-Benzothiazolone was even found in some biological samples (Prawn and bird eggs: ~20 – 300 ng/g f.w.).

Branched alkylated benzenes

The group of branched alkylated benzenes (BABs) are found with a long list of individual compounds in sewage samples (ΣBABs ~ 20 – 50 ng/g d.w.). These petrochemical products are used in chemical synthesis, surfactant industry, as plasticizers, solvents, and metal cutting oils.

6.2.4 Phthalates/adipates

The findings of phthalates, an important group of plasticizers, in nearly all samples is as expected (air: up to 6 ng/m3; sewage/sediment: up to 100 ng/g d.w.; influent/effluent: up to 1,5 µg/L). In some cases especially in the contaminated sediment also other plasticizer like adipates were found (up to 100 ng/g d.w.).

6.2.5 Pesticides

The following pesticides are found with a reasonable high score factor in the Birkenes air sample which can indicate some atmospheric long range transport potential: Aldimorph (CAS 1704-28-5) and Tridemorph (CAS 24602-86-6), both are used as fungicides. In the air sample from Kjeller we found also the related compound Dodemorph (CAS 1593-77-7). These class of fungicides were also found in effluent from the VEAS STP. As these measurements were made by LC-MS, no concentration could be estimated.

6.2.6 Halogenated compounds

A lot of different halogenated compounds were found in the sediments from the Grenland area, which is the direct consequence of the emission of a multitude of different organochlorines from Hydro's earlier magnesium plat using elemental chlorine as a reaction medium. (Sum of identified organochloro compounds: at least 200 ng/g d.w.)

Other samples with a high number and concentration of organochlorine compounds are the biological samples of higher trophic level (cod liver and bird eggs). In the Herring gull sample 41 different organochlorines (mainly pesticides and PCBs) were identified. This can be attributed to both bioaccumulation and metabolization of interfering compounds which in other samples would mask this group of compounds by much higher signals.

The per- and polyfluorinated compounds which are of very interest, were quite difficult to detect by this non-target screening approach and only a few findings with a very modest score factor were made in STP influent sample and the prawn sample. One reason may be due to the solvents selected in this study which probably is not optimal for this compound group. The other reason is found in the mono-isotopic nature of fluorine. Both chlorine and bromine are naturally existing with two different isotopes and thus have two different atomic masses (Cl: 35 amu, 76% and 37 amu, 24 %, Br: 79 amu, 51 % and 81 amu, 49 %). This gives a very distinct mass spectral pattern for all ions containing these two atoms. Fluorine, however, has only one stable isotope (19 amu) and there is no easy detectable "fluorine" pattern in a mass spectrum.

6.3 Sample characteristics

6.3.1 Air samples

Not very surprising the remote air sample shows a low number of identified environmental contaminants. However, even in this sample it was possible to detect a number of phthalates and one adipate, a remarkable number of polymer additives, three organophosphates and some fungicides of the morpholine family. Some of these compounds seems to be quite ubiquitous and have been discussed in chapter 6.2. A number of pharmaceuticals were found in both the urban and the remote air samples, which may surprise when taking into account the water-bound nature and application of these pharmaceutical compounds. The semi-urban air sample from NILUs back yard showed the same compound groups represented, however, with more identified compounds in each group. Especially, the group of PACs was more prominent compared to the remote sample.

6.3.2 Samples from sewage treatment plant

In the two sludge samples taken at the start of the sludge digestion and at the end of the sludge digestion the highest number of compounds could be identified for most of the compound classes. Since all central hospitals of Oslo and more than 500 000 people are emitting to VEAS the number of identified pharmaceuticals and personal care products are not really surprising. Also the list of technical compounds is tremendous and contains a lot of compounds which hitherto were not under special focus.

A matter of concern is that the final digested sludge sample was still heavily contaminated. In this sample type which is used as a soil or fertilizer there were found phthalates, organophosphates, polymer additives, PPCPs, many different aromatics, PACs and halogenated compounds.

Also in influent and effluent samples from VEAS a huge number especially of the more water soluble compounds were found. The effluent water sample contains phthalates, organophosphates, polymer additives, PACs, halogenated compounds, and an extreme number of PPCPs.

It may surprise that the total number of compounds found, is higher in the digested sludge and the effluent sample compared to the raw sludge and influent sample. However, this observation is in all likelihood not reflecting reality, but must be attributed to a much higher total organic content in the extract, which are causing so called ion suppression in the mass spectrometer and result in a considerable reduced instrumental sensitivity.

6.3.3 Sediment sample

With its origin from the heavily industrial polluted Grenland area this sediment sample is not typical for the Norwegian environment. Both the number of identified compounds and the tentatively determined concentrations would be expected from a sewage sample (e.g. emission sample) not from a sample of the outer environment. It contained the longest list of phthalates and adipates found in this study. Also different benzothiazoles, benzotriazole, and antioxidants all used in technical products were detected. As known from earlier monitoring studies the list of polycyclic aromatic compounds (PACs) were long with more than 90 detected compounds of this group. Last but not least also a group of different chlorinated and brominated compounds were identified with remarkable concentrations.

The detected compound classes and extreme concentrations are truly reflecting the historical emissions to this fjord area, where the chlorinated compounds can roughly be attributed to a abandoned magnesium plant (Norsk hydro) and the PACs to former emissions from a ferro-manganese plant (Elkem now Eramet).

6.3.4 Biota samples

The number of identified compounds in the biota samples were much lower than in the before mentioned samples. However, the number of PPCP compounds (only pharmaceuticals!) detected by LC-MS methods are astonishing high. As pharmaceuticals by their nature are very similar to or even identical with natural compounds, there may be a high or very high number of natural compounds remaining in this list of pharmaceuticals.

Since the samples were taken in an accidental manner at several different sites with very a different general contamination pattern, the results must be discussed with some caution. However, it is obvious that many of the compounds identified in the samples of the abiotic environment either will not be bioaccumulated at all or may be metabolized and excreted by the studied animals. Many of the typical bioaccumulating compounds could be identified. Not very surprising this included also a long list of different halogenated compounds, including the chlorinated pesticides p,p'-DDE (~2 – 50 ng/g f.w.) and DDMU (~ 3 ng/g f.w.), chlordanes (Σ ~50 ng/g f.w.), toxaphenes (~10 ng/g f.w.) Mirex and photo-Mirex (~15 ng/g f.w.), but also other pesticides like atrazines (LC-MS, not quantified).

The prawn sample which is an organism on the lower level of the food chain and with limited metabolic power, showed a heavy load of different PACs (Σ ~ 300 ng/g f.w.).

7. Conclusions and recommendations

The main goal of this project was achieved without any deduction, namely to proof that non-target screening is a practical and useful tool for identification of unknown or new emerging environmental pollutants. It was possible to identify huge number of new or earlier unrecognized contaminants in different environmental samples.

The following compound classes were identified and partially quantified in this study: pharmaceuticals and personal care products (PPCP) including perfumes and biocides, polycyclic aromatic compounds (PACs), polymer additives and other compounds used in technical applications including phthalates/adipates, antioxidants, benzothiazoles/triazoles, and branched alkylated benzenes (BABs), pesticides, and halogenated compounds (prevailing chlorinated and brominated compounds).

It was also asked if it is possible to estimate the quantity of the identified compounds in an easy and straightforward way. This is unfortunately only possible for compounds detected by the GC-MS methods. The reason for that is the tremendous variation of ionization potential and hence response in the available LC-MS methods. The only way out of this is to calibrate the LC-MS system with an isolated standard of the compound of interest. That means quantification is in principal possible for all detected compounds, however, in some cases this may be quite complicated, work intensive, and thus also expensive. On the other hand the use of isolated standards is also the most reliable way to finally proof and verify the tentatively identification, and is one of our most important recommendations.

In order to use the full potential of the ToF-MS technique for non-target screening and especially retrospective analysis at a later stage, we strongly recommend to include this analytical technique in future screening and more regular monitoring studies.

We recommend to compare and discuss the list of tentatively identified compounds against what is known about use, environmental occurrence, and environmental and toxic effects.

Before starting more work on risk assessment and potentially regulatory measures we strongly suggest to start the verification of these initial findings by more sophisticated studies. This should include a dedicated sampling strategy either to proof atmospheric long range potential and persistency, or bioaccumulation potential.

To take the full advantage of the data and knowledge generated during this study and to stimulate the national and international research in this field we suggest to report the verified data into the databases of the European network of laboratories monitoring emerging pollutants (NORMAN).

8. References

Arp, H.P., Møskeland, T. and Volan, C. (2012) Drammensfjord - Screening for "nye" miljøgifter 2011. Oslo, NGI

Bastos, P.M. and Haglund, P. (2012) The use of comprehensive two-dimensional gas chromatography and structure-activity modeling for screening and preliminary risk assessment of organic contaminants in soil, sediment, and surface water. *Journal of Soils and Sediments, 12*, 1079-1088.

Muusse, M., Langford, K., Tollefsen, K.E., Cornelissen, G., Haglund, P., Hylland, K. and Thomas, K.V. (2012) Characterization of AhR agonist compounds in roadside snow. *Analytical and bioanalytical chemistry, 403*, 2047-2056.

Rostkowski, P., Horwood, J., Shears, J.A., Lange, A., Oladapo, F.O., Besselink, H.T., Tyler, C.R. and Hill, E.M. (2011) Bioassay-Directed Identification of Novel Antiandrogenic Compounds in Bile of Fish Exposed to Wastewater Effluents. *Environmental Science & Technology, 45*, 10660-10667.

Appendix

Remote air GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ adipates					
DEHP	117-81-7	C24 H38 O4	938	Phthalate	3774
Dibutyl phthalate	84-74-2	C16 H22 O4	867	Phthalate	624
Diethyl Phthalate	84-66-2	C12 H14 O4	940	Phthalate	529
Diisooctyl adipate	1330-86-5	C22 H42 O4	869	Adipate	382
Phthalic acid, 2-ethyl hexyl ester	4376-20-9	C16 H22 O4	813	Phthalate	82
Organophosphates					
Triphenyl phosphate	115-86-6	C18 H15 O4 P	751	OP	51
Other polymer additives					
2,6-di-t-butyl-p-benzoquinone	719-22-2	C14 H20 O2	798	Antioxidant	970
Oleyl nitrile	112-91-4	C18 H33 N	906	Plasticizer, OLN	645
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	883	Antioxidant degr. Prod.	192
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	887	Antioxidant	147
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	C15 H22 O2	894	Antioxidant	137
Benzothiazole	95-16-9	C7 H5 NS	835	S-heteo	88
Bayer 28,589	728-40-5	C14 H21 N O3	754	Antioxidant	21
1-Octanethiol	111-88-6	C8 H18S	750	Polymerization regulator	15
PPCP + flavour/fragrances					
Benzophenone	119-61-9	C13 H10 O	822	Ketone	6,3
PAC					
Pyrene	129-00-0	C16 H10	851	PAC	16

Remote air LC-MS

Name	CAS	Formula	Similarity	Class
OP				
Ethanol, 2-butoxy-, phosphate (3:1)		C18 H39 O7 P	681	OP
Tributyl phosphate or triisobutyl phosphate		C12 H27 O4 P	711	OP
Triphenyl phosphate		C18 H15 O4 P	990	OP
Biocides				
Aldimorph	1704-28-5	C18 H37 N O	998	Fungicide
Hexazinone	51235-04-2	C12 H20 N4 O2	613	Herbicide
Irgarol	28159-98-0	C11 H19 N5 S	619	algicide, antifouling
Tridemorph	24602-86-6	C19 H39 N O	998	Fungicide
Phthalates				
benzyl butyl phthalate		C19 H20 O4	781	phthalate
dibutyl phthalate		C16 H22 O4	972	phthalate
diethyl phthalate		C12 H14 O4	982	phthalate
Dioctyl phthalate or diethylhexyl phthalate (DEHP)		C24 H38 O4	980	phthalate
Other polymer components/additives				
Oleamide		C18 H35 N O	971	Lupricant, slip agent
dicyclohexylamine (DCHA)		C12 H23 N	855	benzenediamine
Benzothiazole		C7 H5 N S	894	benzothiazole
Di(benzothiazole-2-yl)disulphide (DBD)		C14 H8 N2 S4	987	benzothiazole
Fragrances				
Hexyl dodecanoate	34316-64-8	C18 H36 O2	994	
Ethenzamide	938-73-8	C9 H11 N O2	820	Analgesic
Amafolone	50588-47-1	C19 H31 N O2	981	Antiarrhythmic
Nor-Cyclizine	841-77-0	C17 H20 N2	769	Antihistamine
Oxatomide	60607-34-	C27 H30 N4 O	734	Antihistamine

Name	CAS	Formula	Similarity	Class
Etisazole	3 7716-60-1	C9 H10 N2 S	977	Antimycotic
Etaminil	15599-27-6	C15 H22 N2	463	Antitussive
Flavoxanthin	512-29-8	C41 H58 O3	741	Biomolecule
Cassaidine	26296-41-3	C24 H41 N O4	927	Cardiotonic
Cassaidine	26296-41-3	C24 H41 N O4	897	Cardiotonic
Ramnodigin	33156-28-4	C29 H44 O6	693	Cardiotonic
Dicirenone	41020-79-5	C26 H36 O5	880	Diuretic
Dicirenone	41020-79-5	C26 H36 O5	902	Diuretic
Nor-iso-LSD	71953-76-9	C19 H23 N3 O	671	hallucinogen metabolite
Azimexone	64118-86-1	C9 H14 N4 O	848	Immuno modulator
Hydroxyprogesterone caproate	630-56-8	C27 H40 O4	790	Progestin; synonym = 17-Hydroxyprogesteroncaproat
Mexiprostil	88980-20-5	C23 H40 O6	912	Prostaglandin
Fencamine	24356-67-0	C20 H28 N6 O2	760	Psychotropic
2-Benzyltetronic acid	3734-22-3	C11 H10 O3	714	solubilizer for aminophenazone
Cyprodenate	15585-86-1	C13 H25 N O2	993	Stimulant
Octodrine	543-82-8	C8 H19 N	880	Sympathomimetic
Alprostadil	745-65-3	C20 H34 O5	905	Vasodilator
Estriol triacetate	2284-32-4	C24 H30 O6	996	
Laberalol		C19 H24 N2 O3	734	
Phenylbutazone		C19 H20 N2 O2	601	NSAID
Sulfacetamide		C8 H10 N2 O3 S	470	
Triamcinolone		C21 H27 F O6	540	

Name	CAS	Formula	Similarity	Class
Miscellaneous				
3-Pyridinepropionic acid		C8 H9 N O2	850	
Benzimidazole		C7 H6 N2	563	
Butyl 4-aminobenzoate		C11 H15 N O2	476	
Chenodeoxycholic acid		C24 H40 O4	709	
Not identified				
		C5 F2 O2	776	
		C20 H42 O5	999	
		C20 H39 N O	998	
		C24 H47 F3 O5	998	
		C20 H37 N O	998	
		C22 H43 F3 O4	997	
		C29 H65 F N6 O11	997	
		C31 H2 Cl2 F4 N O6 S	997	
		C30 H59 F3 O8	997	
		C25 H45 N	997	
		C6 H15 N O	996	
		C24 H3 Cl2 F7 N2 O S	996	
		C19 H38 O5	995	
		C31 H62 F3 N2 O5	995	
		C34 H68 N6 O11	995	
		C40 H82 N2 O2	995	
		C20 H37 N O	995	
		C22 H42 O4	995	
		C19 H Cl2 F5 N8 O2 S3	994	
		C41 H55 F N5 O3	994	
		C13 H22 O2	994	
		C18 H38 O4	994	
		C26 H52 F3 N2 O2	994	
		C20 H33 F N7	994	
		C24 H47 N O	993	

Name	CAS	Formula	Similarity	Class
		C33 H66 F3 N2 O6	993	
		C20 H41 N O	993	
		C28 H40 O3	993	
		C25 H35 N O2 S3	992	
		C22 H41 F3 N	992	
		C33 H71 F4 N12 O4	992	
		C22 H46 O6	992	
		C27 H59 F N6 O8	992	
		C26 H51 F3 O6	992	
		C31 H62 F4 N3 O3 S2	991	
		C29 H62 F N15 O3	991	
		C27 H49 N	991	
		C13 H16 N2 O3 S2	991	
		C31 H67 F4 N12 O3	991	
		C29 H58 F3 N2 O4	991	
		C24 H50 O7	991	
		C19 H10 Cl2 N8 O4	991	
		C20 H36 N4	991	
		C26 H52 F3 N2 O2	991	
		C23 H49 N O7	990	
		C20 H43 N O5	990	
		C17 H29 N O	990	
		C17 H42 F N8 O	990	
		C17 H40 F N8 O2	990	
		C23 H54 F N8 O4	990	
		C22 H41 F3 O5	990	
		C36 H62 F3 N2 O5	990	
		C19 H37 F3 O2	989	
		C17 H36 O3	989	
		C17 H25 F3 O7	989	
		C18 H41 F N6 O6	989	
		C16 H34 O3	988	
		C17 H36 O3	988	

Name	CAS	Formula	Similarity	Class
		C15 H9 F5 N3	988	
		C37 H63 F3 O8	987	
		C20 H48 F2 N9 O S2	987	
		C30 H61 N8 O5	987	
		C24 H56 F2 N9 O3 S2	987	
		C27 H54 F3 N2 O3	986	
		C19 H46 F N8 O2	986	
		C39 H79 N8 O10	986	
		C24 H45 F3 O6	986	
		C18 H4 Cl2 F2 N7 O7 S	986	
		C9 H18 N2	986	
		C21 H37 N O2	986	
		C20 H35 N O	985	
		C42 H55 F N6	985	
		C32 H65 N8 O6	984	
		C17 H37 N O2	984	
		C10 H20 O4	984	
		C16 H35 N O2	984	
		C20 H39 N O	983	
		C11 H9 F N2 O S3	983	
		C38 H61 F6 N3	983	
		C17 H38 F2 N3 S	983	
		C21 H41 F3 O3	983	
		C22 H43 N O	983	
		C37 H51 F N2 O4	982	
		C27 H45 F3 O5	982	
		C23 H37 F3 O3	981	
		C8 H4 O3	981	
		C25 H55 F N6 O7	981	
		C40 H58 F2 N6 O	980	
		C19 H40 O4	980	
		C34 H47 Cl F N O S4	980	

Name	CAS	Formula	Similarity	Class
		C31 H46 F O4	979	
		C41 H79 N8 O7	979	
		C14 H20 F4 N	978	
		C28 H55 N8 O5	978	
		C10 H10 N2 O S3	978	
		C31 H69 F2 N11 O S	978	
		C21 H37 N	978	
		C18 H38 N9 O2 S	978	
		C23 H41 N	978	
		C11 H9 F N2 O S4	978	
		C25 H49 F3 O5	978	
		C26 H46 F4	975	
		C46 H80 N10 O9	974	
		C21 H41 F3 O3	974	
		C26 H55 F2 N5 O2 S	973	
		C7 H9 Cl N2 O2 S4	971	
		C27 H50 Cl F2 N O S3	971	
		C33 H74 F N21 O3	971	
		C23 H19 Cl2 F N5 O	971	
		C27 H53 F3 O6	970	
		C17 H28 Cl N3 O2 S4	970	
		C27 H24 Cl2 F N4 O3	969	
		C27 H20 Cl2 F N4 O3	969	
		C25 H56 F2 N6 O4 S	968	
		C27 H22 Cl2 F N4 O3	967	
		C27 H58 F2 N3 O5 S	967	
		C27 H24 Cl2 F N4 O3	966	
		C29 H22 Cl2 F N O4	966	
		C38 H77 N O10	966	

Name	CAS	Formula	Similarity	Class
		C8 H14 F4 N O	966	
		C9 F2 N2 O5 S2	965	
		C7 H9 Cl N2 O2 S4	965	
		C25 F13 N4 O5	965	
		C11 H7 Cl N2 O2 S4	964	
		C45 H71 F2 O7	964	
		C32 H71 F N6 O5 S2	963	
		C34 H66 F4 O5	963	
		C26 F11 N2 O7	962	
		C28 H51 Cl F N S4	961	
		C29 H62 F2 N3 O6 S	961	
		C26 H58 F6 N14	961	
		C7 H9 Cl N2 O3 S4	961	
		C22 H48 F N11 O2	960	
		C20 H Cl2 F4 O	959	
		C7 H12 Cl N O2 S3	959	
		C13 H10 Cl N3 O2 S4	957	
		C24 H40 F4 N	957	
		C25 H46 Cl F2 N O S3	957	
		C28 H51 Cl F N S4	957	
		C17 H38 F2 N3 S	956	
		C36 H60 N3 O9	956	
		C6 H7 Cl N2 O2 S4	956	
		C10 H18 Cl F2 N S4	955	
		C21 H41 N8 O	954	
		C27 H55 N8 O	954	
		C26 H F8 N8 O8	952	
		C6 H8 F N O3 S3	952	
		C36 H68 F N8 S	951	
		C31 H67 F4 N15	950	
		C28 H48 N3 O6	950	
		C9 H Cl F2 N6 S5	950	

Name	CAS	Formula	Similarity	Class
		C29 H47 Cl F N S3	949	
		C42 H65 N5 O S	949	
		C10 Cl2 N O9	945	
		C15 H38 F N8	942	
		C25 H F10 N10 O6	941	
		C24 H51 N O7	941	
		C28 H6 Cl2 N3 O9 S4	940	
		C21 H44 O4	939	
		C7 H10 Cl N6 O S4	932	
		C28 H62 N2 O4 S2	930	
		C28 H63 F2 N8 O2 S	928	
		C14 H36 N5 O4 S	928	
		C25 H37 N O2 S3	923	
		C27 H58 F4 N12 O2	921	
		C7 H10 Cl N6 O S4	920	
		C36 H66 F2 O S3	917	
		C30 H47 N5	917	
		C25 H55 N14	916	
		C16 H39 F N8 O2 S	914	
		C18 H40 N3 O3	913	
		C41 H84 F N O8 S	913	
		C9 H18 N2 O	906	
		C35 H74 F N21 O2	904	
		C29 H62 F4 N12 O3	901	
		C59 H73 N13 O	899	
		C22 H48 F2 N6 S	898	
		C22 H40 N3 O4	894	
		C26 H55 F N2 O4 S	888	
		C13 H25 N O3	884	
		C30 H61 F3 N3 O7 S	883	
		C9 H12 N8	882	
		C58 H73 N9 O4	876	
		C37 H42 F N2 O2	874	

Name	CAS	Formula	Similarity	Class
		C29 H61 N O6	869	
		C8 H4 O3	861	
		C13 Cl2 N2 O	858	
		C21 H40 F3 N2	854	
		C22 H43 F3 O2	849	
		C18 H47 F3 N13 O2	848	
		C18 H34 F4 N7	844	
		C26 H59 F2 N8 O S	843	
		C22 H43 F3 O2	841	
		C25 H42 F6 N	838	
		C36 H79 N17 S2	836	
		C7 H10 N4	834	
		C15 H42 F2 N18	833	
		C22 H44 N6 O3	833	
		C13 H20 O2	833	
		C H Cl F O4	829	
		C21 H53 F2 N15 O	829	
		C27 H44 F2 O	828	
		C6 H12 N2 O7	828	
		C27 H54 F2 O2 S	824	
		C27 H57 N O5	821	
		C20 H51 F3 N13 O3	817	
		C17 H47 F5 N15	817	
		C30 H66 F N4 O3 S	817	
		C16 F N2 O18 S	814	
		C25 H42 N10	813	
		C27 H38 F2 N7 O	812	
		C24 H52 F4 N12 O	811	
		C13 H14 N2 O7	803	
		C25 H42 F2 N2 O4	802	
		C18 H3 F22 N2 O	797	
		C19 H3 F20 O3	796	
		C25 H54 F6 N11	796	
		C25 H44 F4 N4 O2	795	

Name	CAS	Formula	Similarity	Class
		C30 H60 F3 N5 O	793	
		C22 H42 N14 O3	779	
		C31 H62 F4 N7	779	
		C7 H5 N5 O6	770	
		C25 F N3 O16	767	
		C23 H47 N8	764	
		C16 H5 F6 N5 O16	759	
		C12 H13 N3 O2	756	
		C7 H6 N4 O3 S	749	
		C32 H28 N2 S3	747	
		C33 H59 F7 N5	747	
		C9 H F O	746	
		C35 H37 N3 S4	735	
		C38 H43 N3 S5	734	
		C30 H47 F3 N4	732	
		C8 H24 N6 O S	723	
		C7 N O6 S	719	
		C46 H29 Cl F N10	709	
		C36 H60 N13	705	
		C9 H8 N4 O3	704	
		C15 H9 N O2	703	
		C14 H4 N4 O11	699	
		C17 H20 N2	694	
		C15 H N3 O	687	
		C10 H17 N3 O S	686	
		C29 H36 F2 N2 O2 S4	684	
		C33 H40 O	682	
		C40 H68 N2 O5	676	
		C5 H5 N5 S3	676	
		C8 H5 N3 O6	673	
		C12 H8 O8	669	
		C6 H12 N2 O7	669	
		C9 H25 N5 O3	663	

Name	CAS	Formula	Similarity	Class
		C14 H24 N2 S	662	
		C21 H45 N17 O3	653	

Urban air GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ adipates					
DEHP	117-81-7	C24 H38 O4	936	Phthalate	119
Dibutyl phthalate	84-74-2	C16 H22 O4	885	Phthalate	31
Diethyl Phthalate	84-66-2	C12 H14 O4	938	Phthalate	16
Benzyl butyl phthalate	85-68-7	C19 H20 O4	881	Phthalate	4,3
Hexanedioic acid, mono(2-ethylhexyl)ester	4337-65-9	C14 H26 O4	781	Adipate	3,9
Organophosphates					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	777	OP	5,0
Triphenyl phosphate	115-86-6	C18 H15 O4 P	719	OP	3,4
Tributyl phosphate	126-73-8	C12 H27 O4 P	793	OP	1,1
Other polymer additives					
Oleyl nitrile	112-91-4	C18 H33 N	894	Plasticizer, OLN	49
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	C14 H20 O2	756	Antioxidant	12
2-Benzothiazolamine, N-ethyl-	28291-69-2	C9 H10 N2 S	826	Benzothiazole	11
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	895	Antioxidant	9,2
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C14 H22 O	867	Antioxidant degr. Prod.; Keto-ester	8,7
2,5,5-Trimethyl-3-hexyn-2-ol	1522-16-3	C9 H16 O	759	Hydroxy-alkyl (used in olifin polymers)	8,4
11-Octadecynenitrile	56599-92-9	C18 H31 N	716	Plasticizer	8,0
Butylated Hydroxytoluene	128-37-0	C15 H24 O	799	Antioxidant	5,4
Benzothiazole	95-16-9	C7 H5 N S	866	Benzothiazole	4,7
2,4,7,9-Tetramethyl-5-decyn-4,7-diol	126-86-3	C14 H26 O2	768	Defoamer (BASF)	2,4
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	826	Plasticizer	2,2
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1522-16-3	C15 H22 O2	784	Antioxidant	1,9
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	704	Benzothiazole	0,8

Name	CAS	Formula	Similarity	Class	ng/sample
PPCP + flavour/fragrances					
Benzophenone	119-61-9	C13 H10 O	732	Ketone, PPCP	2
PAC (isomer often unknown)					
2,6-Diisopropylnaphthalene		C16 H20	705	PAC	1,8
Fluoranthene	206-44-0	C16 H10	786	PAH	4,3
Phenanthrene	85-01-8	C14 H10	754	PAH	2,5
Pyrene	129-00-0	C16 H10	778	PAH	2,4
2,6-Diisopropylnaphthalene		C16 H20	712	Alkyl-PAH	1,6
1,1'-Biphenyl, 2-(phenylmethyl)-	606-97-3	C19 H16	755	PAH	1,3
Triphenylene	217-59-4	C18 H12	788	PAH	0,8
Cyclopenta[cd]pyrene	27208-37-3	C18 H10	777	PAH	0,7
Anthracene	120-12-7	C14 H10	778	PAH	0,0

Urban air LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Dodemorph	1593-77-7	C18 H35 N O	865	Fungicide
Aldimorph	1704-28-5	C18 H37 N O	987	Fungicide
Clofop-isobutyl	51337-71-4	C19 H21 Cl O4	659	Herbicide
Disulfiram	97-77-8	C10 H20 N2 S4	743	AlcoholDeterrent
Clofop-isobutyl	51337-71-4	C19 H21 Cl O4	659	Herbicide
OP				
Tributyl phosphate or triisobutyl phosphate		C12 H27 O4 P	939	OP
Triphenyl phosphate		C18 H15 O4 P	940	OP
Ethanol, 2-butoxy-, phosphate (3:1)		C18 H39 O7 P	964	OP
Tributylphosphate	126-73-8	C12 H27 O4 P	959	Plasticizer
Phthalates				
diethyl phthalate		C12 H14 O4	893	phthalate
benzyl butyl phthalate		C19 H20 O4	951	phthalate
dibutyl phthalate		C16 H22 O4	972	phthalate
Other polymer components/additives				
dicyclohexylamine (DCHA)		C12 H23 N	977	benzenediamine
Benzothiazole		C7 H5 N S	899	benzothiazole
Pharmaceuticals and biomolecules				
Morpheridine	469-81-8	C20 H30 N2 O3	719	Analgesic
Indopine	3569-26-4	C23 H28 N2	887	Analgesic
Pexantel	10001-13-5	C12 H22 N2 O	862	Anthelmintic
Benrixate	24671-26-9	C19 H30 N2 O2	819	Antiarrhythmic
Lovastatin	75330-75-5	C24 H36 O5	825	Anticholesteremic
Dimepregnene	21208-26-4	C23 H36 O2	884	Antiestrogen
Histapyrrodine	493-80-1	C19 H24 N2	758	Antihistamine
Cassaidine	26296-41-3	C24 H41 N O4	890	Cardiotonic
Vanyldisulfamide	119-85-7	C20 H22 N4 O6 S2	657	Chemotherapeutic
Domoprednate	66877-67-6	C26 H36 O5	850	Corticoid
Azelaic acid	123-99-9	C9 H16 O4	835	Dermatic

Name	CAS	Formula	Similarity	Class
Phencyclidine (PCP)	77-10-1	C17 H25 N	660	Hallucinogen, anaesthetic
Azimexone	64118-86-1	C9 H14 N4 O	939	Immuno modulator
Carperone	20977-50-8	C19 H27 F N2 O3	817	Neuroleptic
Cinitapride	66564-14-5	C21 H30 N4 O4	960	Neuroleptic
Deprostil	33813-84-2	C21 H38 O4	880	Prostaglandin
Isovaleric acid	503-74-2	C5 H10 O2	821	Sedative
Cyprodenate	15585-86-1	C13 H25 N O2	990	Stimulant
Not identified				
		C38 H71 F7 N4 O	705	
		C37 H67 F2 N2 O3	706	
		C47 H49 S5	709	
		C44 H43 O S4	713	
		C30 H53 F2 N2	716	
		C10 F5 N2 O11 S3	716	
		C40 H41 F2 O S4	717	
		C10 H14 N2	720	
		C38 H43 N3 S5	727	
		C32 H15 Cl N13 O2	727	
		C32 H57 F2 N2 O	728	
		C35 H37 N3 S4	735	
		C28 H62 F N18	738	
		C36 H39 N3 S4	738	
		C35 H20 F N8 O2 S	739	
		C18 F15 N4 O5	741	
		C24 H28 N7 O S4	743	
		C37 H38 F S4	744	
		C23 H53 N4 O4	747	
		C29 H35 N2 O S4	748	
		C9 H16 N O	749	
		C18 H O16 S2	752	
		C5 H9 N O	753	
		C22 H51 N4 O4	753	

Name	CAS	Formula	Similarity	Class
		C31 H48 F2 N4	754	
		C32 H69 N4 O4	754	
		C2 F4 N2 O4 S	755	
		C27 H46 F2 O2	757	
		C32 H28 N2 S3	757	
		C26 H49 F3 O3	762	
		C15 F9 O9 S2	763	
		C33 H68 F3 N5 O3	763	
		C33 H33 N3 S3	767	
		C8 H4 O3	768	
		C9 H18 S3	770	
		C26 H51 F3 O3	773	
		C20 F3 N O11 S2	774	
		C20 H39 F4 N4 O4	777	
		C17 F17 N6 O3	780	
		C5 H13 N O	784	
		C22 H51 N4 O3	785	
		C26 H17 Cl N7	787	
		C31 H68 F N4 O3 S	788	
		C24 H47 F3 O2	788	
		C9 H18 N2 O	789	
		C39 H70 F2 N4 O3 S	796	
		C27 H46 F2 O2	796	
		C25 H51 N8 O	797	
		C36 H69 F S4	797	
		C23 H47 N8	803	
		C17 H33 F3 O	806	
		C44 H63 F2 N3 O	807	
		C27 H53 F N6 O S	807	
		C13 H13 N4 O S2	808	
		C40 H77 N4 O S	808	
		C21 H53 F3 N13	810	

Name	CAS	Formula	Similarity	Class
		O3		
		C19 H47 F N9 O4	815	
		C24 H52 F4 N12 O	817	
		C20 H36 N4	818	
		C23 H46 N6 O4	818	
		C25 H51 N8	820	
		C15 H42 F2 N18	822	
		C27 H51 N S	823	
		C13 H20 O2	826	
		C6 H10 N3 O3	827	
		C23 H48 F2 N10 O2	827	
		C24 H49 F3 N3 O3	828	
		C36 H71 N18	828	
		C23 H42 N4	829	
		C17 H41 F N9 O2	834	
		C21 H43 F3 N3 O2	834	
		C15 H33 Cl N O3	835	
		C23 H45 F3 O3	837	
		C34 H72 F N14 O S	839	
		C6 H10 N3 O3	839	
		C22 H39 F3 O4	841	
		C34 H69 N21 O	842	
		C21 H44 O4	844	
		C22 H43 F3 O2	845	
		C35 H67 N O3 S	848	
		C19 H29 F3	849	
		C31 H52 N3 O S	852	
		C10 H18 N3 O2	853	
		C38 H75 F2 N O3	853	
		C40 H68 O4 S2	853	
		C27 H39 F5	854	
		C35 H76 N6 O9 S	855	

Name	CAS	Formula	Similarity	Class
		C20 H39 F3 O2	855	
		C10 H12 N3 O4	855	
		C9 H16 N O	860	
		C8 H12 N3 O2	860	
		C37 H71 N O4 S	864	
		C43 H60 F2 N4 O6	865	
		C6 H10 N3 O3	866	
		C9 H16 N3 O3	866	
		C26 H52 F N4 S2	871	
		C43 H85 F N5 O3 S	872	
		C33 H70 F N4 S	873	
		C18 H F4 N O18	875	
		C5 H11 N O2	880	
		C43 H64 F N3	880	
		C45 H71 F2 O7	880	
		C32 H42 F N4	881	
		C37 H77 F N12 O S2	881	
		C30 H45 F O2	881	
		C45 H71 F2 O7	884	
		C39 H82 F N4 O3 S	885	
		C24 H51 N11 O	889	
		C30 H64 F2 N6 S	892	
		C29 H63 F3 N10 O7	896	
		C37 H66 Cl N2 O7 S3	898	
		C26 H55 N11 O	900	
		C38 H69 F2 N2 O3	901	
		C13 H25 N O3	903	
		C32 H59 F2 N5	907	
		C29 H59 F5 N4 O4	907	
		C33 H65 F3 N3 O2	910	

Name	CAS	Formula	Similarity	Class
		C27 H38 N4	911	
		C25 H43 F N3 O S	914	
		C22 H3 F2 N6 O17	915	
		C32 H57 F2 N2	916	
		C29 H61 N11 O2	917	
		C23 H41 N	917	
		C35 H63 F2 N2 O3	918	
		C19 H30 F4 N3 S2	924	
		C21 F5 O16	925	
		C31 H55 F2 N2 O	925	
		C36 H77 F2 N18 S	928	
		C20 H50 N16 O4	929	
		C37 H68 N9 O4	929	
		C22 H47 N11	931	
		C25 F N3 O16	932	
		C31 H60 F N5 S	935	
		C22 H39 F3 O2	937	
		C34 H75 F2 N8 O2 S	938	
		C33 F11 N O4	939	
		C42 H85 N O12	940	
		C25 H43 O S2	941	
		C22 H41 F2 O3 S	942	
		C10 H18 F2 N3 O3 S	944	
		C23 H46 N6 O4	944	
		C42 H75 F5 O8	947	
		C16 H35 N O2	948	
		C8 H19 N	949	
		C33 H64 F N5 S	949	
		C10 H18 N3 O3	949	
		C37 H62 N3 O9	951	
		C24 H49 N8 O2	953	
		C27 H58 F4 N12	953	

Name	CAS	Formula	Similarity	Class
		O2		
		C17 H46 F2 N18 O	955	
		C18 H49 F5 N15	956	
		C29 H55 F N3 O S	958	
		C17 H37 N O2	960	
		C15 H39 F N9 O3	962	
		C12 H27 N O3	963	
		C11 H18 N4	965	
		C17 H37 N O2	965	
		C12 H25 N O	967	
		C8 H14 N O	968	
		C12 H22 N3 O4	968	
		C26 H57 F3 N17 O	969	
		C44 H81 F2 N5 O2	969	
		C12 H27 N O2	970	
		C14 H31 N O2	971	
		C25 H42 F2 N2 O4	972	
		C24 H43 F N6	974	
		C24 H38 O4	974	
		C13 H20 N5	976	
		C14 H31 N O3	976	
		C20 H52 F2 N18 O2	976	
		C16 H34 O3	977	
		C22 H43 N O2	977	
		C34 H72 F2 N6 O2 S	977	
		C7 H12 N3 O3	977	
		C22 H42 O4	977	
		C21 H48 F2 N6 O2 S	977	
		C10 H23 N O	980	
		C38 H77 N O10	980	
		C19 H37 F3 O2	981	

Name	CAS	Formula	Similarity	Class
		C16 H22 O4	981	
		C25 H51 N8 O3	985	
		C22 H44 F3 N2	985	
		C8 H14 N3 O2	985	
		C18 H25 F3 N O4	985	
		C9 H16 N3 O4	985	
		C28 H56 N6 O8	986	
		C19 H37 F3 O2	986	
		C37 H78 F4 N6 O2 S	986	
		C22 H43 N O	987	
		C17 H32 N3 O5	987	
		C21 H31 F3 O9	987	
		C27 H55 N8 O4	988	
		C28 H63 N4 O9	988	
		C12 H22 N3 O3	988	
		C25 H50 F3 N2 O2	989	
		C24 H47 F3 O5	991	
		C13 H24 N3 O3	991	
		C22 H38 F3 N	992	
		C17 H24 N3 O8	992	
		C18 H39 N O3	992	
		C13 H22 O2	993	
		C44 H89 N O13	993	
		C21 H41 F3 O3	993	
		C18 H38 O4	993	
		C19 H40 O4	994	
		C18 H41 F N7 O2	994	
		C22 H45 N8 O	994	
		C39 H57 F5 N3	994	
		C21 H41 F3 O3	995	
		C22 H43 N O2	995	
		C20 H42 O5	998	
		C26 H51 F3 O6	998	

Name	CAS	Formula	Similarity	Class
		C8 H4 O3	998	

Digested sludge GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates					
DEHP	117-81-7	C24 H38 O4	920	Phthalate	149
Dibutyl phthalate	84-74-2	C16 H22 O4	907	Phthalate	59
1,2-Benzenedicarboxylic acid, dicyclohexyl ester	84-61-7	C20 H26 O4	742	Phthalate	78
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	C16 H22 O4	875	Phthalate	27
Diethyl Phthalate	84-66-2	C12 H14 O4	935	Phthalate	18
Benzyl butyl phthalate	85-68-7	C19 H20 O4	743	Phthalate	13
Organophosphates					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	881	OP	44
Octyl diphenyl phosphate	1241-94-7	C20 H27 O4 P	762	OP	15
Triphenyl phosphate	115-86-6	C18 H15 O4 P	713	OP	1,0
Other polymer additives					
Oleyl nitrile	112-91-4	C18 H33 N	901	Plasticizer, OLN	147
p-Dicyclohexylbenzene	1087-02-1	C18 H26	805	Plasticizer, heat transfer media	24
1,2-Ethanediol, dibenzoate	94-49-5	C16 H14 O4	779	Plastics additive, plasticizer (Benzoflex 988)	26
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	719	Benzothiazole	8,2
Disulfide, bis(4-methylphenyl)	103-19-5	C14 H14 S2	762	Disulfide, cross linking agent	7,9
Benzothiazole	95-16-9	C7 H5 N S	868	Benzothiazole	7,6
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	702	Benzothiazole	4,1
Ethanone, 2,2-dimethoxy-1,2-diphenyl-	24650-42-8	C16 H16 O3	894	Plastics additive, UV photoinitiator	1,0
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	888	Antioxidant	24
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	851	Antioxidant degr. Prod.; Keto-ester	21
PPCP + flavour/fragrances					
Benzophenone	119-61-9	C13 H10 O	933	PPCP, UV blocker	780
Tonalid	21145-77-7	C18 H26 O	718	PPCP, Musk fragrance	230
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	5466-77-3	C18 H26 O3	871	PPCP, sunscreen (Escalol 557)	97
á-Ionone epoxide (isomer)	23267-57-4	C13 H20 O2	907	PPCP (rose aroma)	87
Galoxolide	1222-05-5	C18 H26 O	756	PPCP, Musk fragrance	74

Name	CAS	Formula	Similarity	Class	ng/sample
Dihydroactinidiolide	17092-92-1	C11 H16 O2	870	PPCP, fragrance	50
Dodecanamide (lauramide)	120-16-7	C12 H25 N O	856	PPCP, surfactant?	42
Homomenthyl salicylate	52253-93-7	C16 H22 O3	901	PPCP, sunscreen	40
Benzene, 1,1'-(3,3-dimethyl-1-butenylidene)bis-	3910-35-8	C18 H20	832	PPCP, fragrance	25
á-Ionone epoxide (isomer)	23267-57-4	C13 H20 O2	805	PPCP, fragrance (rose aroma)	17
Cedrene	11028-42-5	C15 H24	845	PPCP, fragrance	11
2-Ethylhexyl salicylate	118-60-5	C15 H22 O3	812	PPCP, sunscreen	11
Kaurene	34424-57-2	C20 H32	719	PPCP, fragrance	11
Cedrol	77-53-2	C15 H26 O	799	PPCP, fragrance	8,2
2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-	20194-68-7	C13 H18 O2	810	PPCP, fragrance?	6,3
3-Oxo-á-ionone	98910-85-1	C13 H18 O2	768	PPCP, fragrance?	3,8
Ionone	8013-90-9	C13 H20 O	752	PPCP, fragrance (rose aroma)	3,4
Halogenated compounds/ Pesticides					
1,1'-Biphenyl, 4,4'-dichloro-		C12 H8Cl2	702	PCB	23
Methanone, (2-chlorophenyl)phenyl-	5162-03-8	C13 H9Cl O	876	Halogenated compound	11
Benzoic acid, 2,4-dichloro-	50-84-0	C7 H4Cl2 O2	637	Halogenated compound	4,5
Benzene, 1,1'-(dichloromethylene)bis-	2051-90-3	C13 H10Cl2	778	Halogenated compound	2,7
Benzenamine, 2,4-dichloro-	554-00-7	C6 H5Cl2 N	714	Halogenated compound	2,2
1,1'-Biphenyl, 2,3',4-trichloro-	55712-37-3	C12 H7Cl3	892	PCB	2,6
Permethrin	51877-74-8	C21 H20Cl2 O3	768	Pesticide	21
Amides					
8-Methyl-6-nonenamide		C10 H19 N O	764	Amide	196
2-Pyrrolidinone, 1-(3,7,11,15-tetramethylhexadecyl)-		C24 H47 N O	771	Amide	95
Alkyl-benzenes					
Benzene, (1-butyloctyl)-	2719-63-3	C18 H30	848	Alkylbenzene, branched (BAB)	23
Benzene, (1-butylheptyl)-	4537-15-9	C17 H28	871	Alkylbenzene, branched (BAB)	19
Benzene, (1-propylnonyl)-	2719-64-4	C18 H30	901	Alkylbenzene, branched (BAB)	9,7
Benzene, (1-methylundecyl)-	2719-61-1	C18 H30	846	Alkylbenzene, branched (BAB)	9,7
Benzene, (1-propyloctyl)-	4536-86-1	C17 H28	861	Alkylbenzene, branched (BAB)	9,6
Benzene, (1-methyldecyl)-	4536-88-3	C17 H28	889	Alkylbenzene, branched (BAB)	8,5
Benzene, (1-ethylnonyl)-	4536-87-2	C17 H28	838	Alkylbenzene, branched (BAB)	7,5
Benzene, (1-ethyldecyl)-	2400-00-2	C18 H30	852	Alkylbenzene, branched (BAB)	6,3
Benzene, (1-propyldecyl)-	4534-51-4	C19 H32	841	Alkylbenzene, branched (BAB)	6,0

Name	CAS	Formula	Similarity	Class	ng/sample
Benzene, (1-butylhexyl)-	4537-11-5	C16 H26	828	Alkylbenzene, branched (BAB)	5,0
Benzene, (1-propylheptyl)-	4537-12-6	C16 H26	790	Alkylbenzene, branched (BAB)	4,4
Benzene, (1-methylnonyl)-	4537-13-7	C16 H26	803	Alkylbenzene, branched (BAB)	2,9
Benzene, butyl-	104-51-8	C10 H14	835	Alkylbenzene, branched (BAB)	1,4
Benzene, 2-ethenyl-1,3,5-trimethyl-	769-25-5	C11 H14	793	Alkylbenzene, branched (BAB)	1,2
PAC					
Fluoranthene	206-44-0	C16 H10	872	PAH	47
Naphthalene, 1-(phenylmethoxy)-	607-58-9	C17 H14 O	802	O-PAH	39
Pyrene	129-00-0	C16 H10	891	PAH	37
Phenanthrene	85-01-8	C14 H10	954	PAH	35
3,4'-Diisopropylbiphenyl		C18 H22	793	Alkyl-PAH	19
9H-Fluorene, 2,3-dimethyl-		C15 H14	839	Alkyl-PAH	21
Pyrene, 1-methyl-		C17 H12	780	Alkyl-PAH	16
9H-Fluorene, 2,3-dimethyl-		C15 H14	717	Alkyl-PAH	16
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-		C15 H18	825	Alkyl-PAH	16
Phenanthrene, 3,6-dimethyl-		C16 H14	799	Alkyl-PAH	15
2,6-Diisopropylnaphthalene		C16 H20	781	Alkyl-PAH	15
2,6-Diisopropylnaphthalene		C16 H20	862	Alkyl-PAH	13
Fluorene	86-73-7	C13 H10	860	PAH	13
Phenanthrene, 1-methyl-		C15 H12	869	Alkyl-PAH	12
2,8-Dimethyldibenzo(b,d)thiophene		C14 H12 S	768	S-heterocyclic	12
4H-Cyclopenta[def]phenanthrene	203-64-5	C15 H10	800	PAH	11
2,6-Diisopropylnaphthalene		C16 H20	869	Alkyl-PAH	11
2,6-Diisopropylnaphthalene		C16 H20	853	Alkyl-PAH	9,9
Phenanthrene, 2-methyl-		C15 H12	897	Alkyl-PAH	9,7
Naphthalene, 1,4,6-trimethyl-		C13 H14	824	Alkyl-PAH	9,7
9H-Fluoren-9-one, 2,3-dimethyl-		C15 H14	706	Oxy-PAH	9,4
Benz[a]anthracene	56-55-3	C18 H12	860	PAH	7,9
Benzo[b]naphtho[2,1-d]thiophene	239-35-0	C16 H10 S	705	S-heterocyclic	7,6
9H-Fluorene, 9,9-dimethyl-		C15 H14	761	Alkyl-PAH	7,2
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	804	Alkyl-PAH	6,7
Naphthalene, 1,4,6-trimethyl-		C13 H14	824	Alkyl-PAH	6,6
Benzo[ghi]fluoranthene	203-12-3	C18 H10	816	PAH	6,3
9,10-Anthracenedione	84-65-1	C14 H8 O2	789	O-PAH	6,3
Dibenzofuran	132-64-9	C12 H8 O	790	O-PAH	6,2

Name	CAS	Formula	Similarity	Class	ng/sample
Naphtho[2,1-b]thiophene	233-02-3	C12 H8 S	747	S-heterocyclic	6,0
Naphthalene, 1,4,6-trimethyl-		C13 H14	807	Alkyl-PAH	5,3
Anthracene, 9-methyl-		C15 H12	829	Alkyl-PAH	4,9
2-Hydroxyfluorene	2443-58-5	C13 H10 O	706	Oxy-PAH	4,5
1H-Indene, 1-(phenylmethylene)-	5394-86-5	C16 H12	804	PAH	3,7
Naphthalene, 2,3-dimethyl-		C12 H12	808	Alkyl-PAH	3,3
Benzo[h]cinnoline	230-31-9	C12 H8 N2	743	N-heterocyclic	3,0
2,6-Diisopropylnaphthalene		C16 H20	815	Alkyl-PAH	2,9
11H-Benzo[a]fluoren-11-one	479-79-8	C17 H10 O	744	O-PAH	2,9
Phenanthrene, 4,5-dimethyl-		C16 H14	702	Alkyl-PAH	2,6
1(2H)-Acenaphthylenone	2235-15-6	C12 H8 O	707	O-PAH	2,4
2-Phenylnaphthalene	35465-71-5	C16 H12	805	PAH	2,3
Naphtho[2,3-b]thiophene	268-77-9	C12 H8 S	748	S-heterocyclic	2,3
Biphenylene	259-79-0	C12 H8	760	PAH	2,2
o-Terphenyl	84-15-1	C18 H14	779	PAH	2,1
Benz(A)anthracene-7,12-dione	2498-66-0	C18 H10 O2	709	O-PAH	1,6
1,1'-Biphenyl, 4-methyl-		C13 H12	804	Alkyl-PAH	1,5
Acenaphthene	83-32-9	C12 H10	720	PAH	1,1
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	803	Alkyl-PAH	1,0
9H-Xanthene	92-83-1	C13 H10 O	753	O-PAH	0,5
Ethanedione, diphenyl-		C14 H10 O2	759	O-PAH	0,4

Digested sludge LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Fluometuron		C10 H11 F3 N2 O	701	Herbicide
Glyphosate		C3 H8 N O5 P	635	Herbicide
Pharmaceuticals and biomolecules				
1(3)-glyceryl-PGF2alpha		C23 H40 O7	921	
1alpha-hydroxy-24-methylvitamin D2 / 1alpha-hydroxy-24-methylergocalciferol		C29 H46 O2	858	
2-heptadecylenic acid		C17 H32 O2	973	
2R-aminohexadecanoic acid		C16 H33 N O2	956	
5-Butyl-5-phenyl-hydantoin		C13 H16 N2 O2	735	Anticonvulsant
Allopregnanediol		C21 H36 O2	978	Hormone
Bencyclane		C19 H31 N O	965	Vasodilator; synonym = Bencyclan
C17 Sphingosine		C17 H35 N O2	988	
C8 Ceramide		C26 H51 N O3	993	
Cetaben		C23 H39 N O2	903	Anticholesteremic
Demissidine		C27 H45 N O	986	
Dihydroceramide C2		C20 H41 N O3	984	Pubchem 6610273
Dimantine		C20 H43 N	993	Anthelmintic
Dimepranol		C5 H13 N O	998	Virucide
Glucosylsphingosine		C24 H47 N O7	959	
Hexyl dodecanoate		C18 H36 O2	977	
His Leu		C12 H20 N4 O3	955	
Ile Glu Thr		C15 H27 N3 O7	835	
Ile Ile		C12 H24 N2 O3	969	
Isomylamine		C18 H35 N O2	976	Muscle relaxant
Leu Val		C11 H22 N2 O3	886	
Lys Lys Met		C17 H35 N5 O4 S	811	
Madecassic acid		C30 H48 O6	754	wound therapeutic
Mephenesin carbamate		C11 H15 N O4	857	Muscle relaxant
Metomidate		C13 H14 N2 O2	765	Hypnotic
Nalidixic acid		C12 H12 N2 O3	811	Chemotherapeutic

Name	CAS	Formula	Similarity	Class
N-Butylamphetamine		C13 H21 N	837	Sympathomimetic
Octamylamine		C13 H29 N	949	Parasympatholytic
Oxaceprol		C7 H11 N O4	748	Antirheumatic
Palmidrol		C18 H37 N O2	989	Antiphlogistic
Phytanic acid		C20 H40 O2	989	Biomolecule
Pirimicarb		C11 H18 N4 O2	959	Insecticide
Promestriene		C22 H32 O2	979	Corticoid
Salinomycin		C42 H70 O11	827	Coccidiostatic
Stevaladil		C27 H45 N O4	981	Cardiotonic
Testosterone dipropionate		C25 H36 O4	773	Androgen
Tocainide		C11 H16 N2 O	673	Antiarrhythmic
Val Leu Val		C16 H31 N3 O4	967	
		C13 H N2 O11	638	
		C23 H41 N2 O6	645	
		C7 H5 N3 O9	656	
		C25 H54 N2 O7	670	
		C40 H77 N2 O9	675	
		C13 H11 O9	677	
		C37 H73 N5 O8	689	
		C34 H67 N5 O5	710	
		C30 H66 N2 O12	718	
		C39 H43 N2 O	725	
		C15 H18 O13	726	
		C29 H58 N4 O4 S	726	
		C20 H3 N2 O16 S3	730	
		C9 H10 N O10	732	
		C36 H62 N4 O6	734	
		C23 H3 N O18 S2	735	
		C19 H38 N5 O S	736	
		C39 H43 N2 O	737	
		C34 H64 O9	737	
		C34 H64 O9	738	
		C35 H67 N2 O6	740	
		C52 H99 Cl N O13	742	

Name	CAS	Formula	Similarity	Class
		C16 H25 N2 O2	743	
		C18 H O20 S2	745	
		C34 H65 N2 O7	746	
		C33 H65 N5 O5	756	
		C22 H44 N2 O	761	
		C32 H52 N O4	763	
		C15 H4 N O2	768	
		C15 H6 N O9	770	
		C14 H29 N O6 S	789	
		C24 H N3 O19 S	801	
		C13 H8 N2 O2	813	
		C23 H45 N2 O7 S	817	
		C31 H57 N5 O10 S	817	
		C26 H53 N O12 S	820	
		C31 H58 O8	822	
		C24 H51 N4 O3	822	
		C24 H49 N O11 S	823	
		C28 H57 N O13 S	824	
		C11 H26 N2 O5	828	
		C13 H8 N2 O2	830	
		C16 H25 N2 O5	831	
		C20 H43 N O3	835	
		C21 H49 N5 O	838	
		C49 H76 O9	843	
		C13 H8 N2 O2	847	
		C27 H52 N3 O7	848	
		C7 H12 N O8	849	
		C39 H76 N3 O11	857	
		C45 H80 N4 O7	858	
		C30 H60 O S2	867	
		C4 H4 Br N O4 S2	875	
		C19 H39 N5 O5 S	877	
		C27 H56 O8	878	
		C20 H38 N5 O5 S	880	

Name	CAS	Formula	Similarity	Class
		C42 H74 N3 O6 S	882	
		C38 H75 N5 O8	884	
		C40 H70 N3 O7 S	886	
		C38 H72 O12	888	
		C23 H43 N3 O11	889	
		C39 H77 N5 O9	893	
		C24 H3 N O24	893	
		C42 H72 O7 S	896	
		C29 H55 N3 O14	897	
		C28 H57 N O4	900	
		C29 H58 N4 O4 S	902	
		C H5 Cl N2 O2 S	903	
		C36 H69 N2 O4	903	
		C25 H47 N3 O12	903	
		C32 H63 N5 O6	904	
		C43 H42 N O2	908	
		C31 H60 N3 O9	914	
		C30 H67 N4 O10	915	
		C37 H72 N3 O11	916	
		C40 H78 N2 O8 S2	917	
		C46 H72 N2 O5	919	
		C30 H60 N3 O3 S2	920	
		C28 H53 N2 O3	924	
		C22 H40 N2 O2	924	
		C37 H71 N3 O8	924	
		C38 H40 O4	924	
		C52 H94 N3 O11 S	925	
		C34 H67 N3 O3 S	925	
		C44 H68 N3 O6	926	
		C39 H65 O4	927	
		C20 H39 N O2	930	
		C40 H77 N2 O6	930	
		C24 H42 N O2	932	
		C42 H66 N5 O3	932	

Name	CAS	Formula	Similarity	Class
		C27 H28 Cl N2 O	933	
		C37 H63 N3 O3	934	
		C26 H53 N O4	934	
		C22 H40 N2 O2	934	
		C42 H71 O3	935	
		C55 H101 N4 O9 S	938	
		C22 H50 N4 O2 S	938	
		C26 H49 N2 O3	938	
		C31 H67 N2 O8 S	939	
		C12 H24 N2 O3	939	
		C24 H54 N4 O3 S	941	
		C26 H50 N3 O6	942	
		C33 H55 N3 O	944	
		C36 H60 N O5	944	
		C35 H59 N3 O2	945	
		C24 H42 N O	946	
		C28 H62 N4 O5 S	947	
		C50 H92 N5 O8 S	947	
		C50 H97 N2 O13	947	
		C26 H42 N4 O2	947	
		C32 H62 N3 O9	948	
		C41 H64 N5 O2	948	
		C29 H54 N4 O4	948	
		C41 H38 N O	948	
		C25 H44 N O2	949	
		C33 H52 N2 O	949	
		C32 H64 N4 O4 S	950	
		C44 H86 N O9 S	950	
		C31 H61 N5 O6	951	
		C41 H69 O5	951	
		C38 H74 N3 O12	952	
		C27 H53 N5 O4	952	
		C31 H59 N2 O5	952	
		C39 H77 N5 O5	952	

Name	CAS	Formula	Similarity	Class
		C15 H32 O6	952	
		C35 H59 N3 O2	952	
		C19 H42 N O S	953	
		C43 H84 N3 O13	953	
		C37 H72 N3 O11	954	
		C43 H48 N O3	954	
		C50 H92 N5 O8 S	954	
		C54 H96 N O14	954	
		C34 H67 N5 O5	955	
		C36 H60 N O4	955	
		C22 H43 N O3	956	
		C29 H57 N5 O5	956	
		C47 H74 N2 O5	956	
		C43 H76 N3 O5 S2	958	
		C35 H70 N4 O7 S	958	
		C38 H83 N4 O12	958	
		C24 H46 N3 O8	958	
		C42 H83 N5 O11	959	
		C47 H92 N3 O15	959	
		C35 H69 N5 O7	960	
		C37 H72 N3 O10	960	
		C42 H81 N O7 S	961	
		C47 H84 N3 O8 S2	961	
		C35 H68 N3 O9	962	
		C26 H51 N5 O2	962	
		C18 H43 N4 O4	963	
		C27 H50 O7	963	
		C36 H70 N2 O6 S2	963	
		C36 H70 N2 O6 S2	963	
		C59 H3 N4 O12 S	963	
		C28 H55 N5 O3	963	
		C29 H63 N2 O7 S	963	
		C14 H30 O4	963	
		C21 H44 O4	964	

Name	CAS	Formula	Similarity	Class
		C34 H75 N4 O10	964	
		C18 H37 N O3	964	
		C52 H96 N5 O11 S	964	
		C32 H61 N2 O6	964	
		C44 H78 N4 O10	965	
		C12 H26 O5	965	
		C33 H43 O	965	
		C49 H94 O17	966	
		C53 H92 N O13	966	
		C33 H64 N3 O11	967	
		C24 H43 N3 O3	968	
		C34 H56 N O4	968	
		C40 H79 N5 O10	968	
		C39 H76 N3 O12	969	
		C42 H82 N O9 S	969	
		C50 H97 N2 O13	969	
		C35 H77 N4 O10	969	
		C18 H39 N O2	969	
		C33 H63 N2 O6	969	
		C57 H101 O12	970	
		C35 H77 N4 O10	970	
		C15 H31 N O	970	
		C31 H58 O8	970	
		C51 H89 N3 O9	971	
		C40 H79 N5 O8	971	
		C46 H89 N2 O11	971	
		C29 H57 N5 O11	971	
		C51 H90 N4 O12	971	
		C33 H62 N3 O10	972	
		C27 H53 N5 O5	972	
		C53 H86 N2 O7	972	
		C25 H46 O6	973	
		C26 H46 N O2	973	
		C37 H73 N5 O7	974	

Name	CAS	Formula	Similarity	Class
		C36 H78 N2 O14	974	
		C49 H86 O8 S2	975	
		C38 H75 N5 O9	975	
		C16 H35 N O	975	
		C18 H39 N O	975	
		C46 H80 N3 O10	975	
		C45 H88 N3 O14	975	
		C51 H97 N2 O13	976	
		C18 H38 O6	976	
		C37 H71 N2 O7	976	
		C20 H10 Cl2 N3 O9 S2	977	
		C41 H80 N3 O12	977	
		C28 H50 N O4	978	
		C30 H54 N O5	978	
		C43 H84 N3 O12 S	978	
		C22 H47 N O2	979	
		C24 H50 O7	979	
		C25 H49 N5 O2	979	
		C27 H52 N3 O9	979	
		C45 H87 N2 O8	979	
		C50 H97 N2 O14	979	
		C30 H67 N4 O9	979	
		C45 H88 N3 O13 S	980	
		C30 H58 N3 O15	980	
		C41 H69 O5	980	
		C48 H93 N2 O12	980	
		C24 H44 N4 O	980	
		C27 H52 N2 O8	980	
		C32 H61 N2 O5	981	
		C49 H94 O16	981	
		C55 H99 N3 O11	981	
		C42 H74 N4 O8	981	
		C35 H69 N5 O6	981	
		C29 H56 N2 O9	982	

Name	CAS	Formula	Similarity	Class
		C35 H66 O9	982	
		C36 H75 N O12	982	
		C31 H58 O9	982	
		C8 H14 N3 O4	982	
		C40 H77 N2 O9	983	
		C45 H86 O14	983	
		C40 H74 N4 O9	983	
		C37 H81 N4 O12	983	
		C24 H44 N4 O	983	
		C44 H87 N5 O10	984	
		C26 H50 N3 O6	984	
		C41 H80 N3 O12	984	
		C34 H66 N3 O10	984	
		C42 H83 N5 O10	984	
		C42 H83 N5 O9	984	
		C37 H81 N4 O11	984	
		C20 H43 N O2	985	
		C48 H84 N4 O11	985	
		C16 H34 O5	985	
		C16 H34 O4	985	
		C36 H69 N2 O7	985	
		C48 H93 N2 O12	985	
		C36 H70 N3 O10	986	
		C22 H46 O12	986	
		C39 H76 N3 O13	986	
		C37 H72 N3 O12	986	
		C47 H90 O15	986	
		C41 H81 N5 O6	986	
		C43 H79 N3 O11	986	
		C40 H88 N4 O14	986	
		C32 H62 N3 O16	986	
		C30 H62 O11	986	
		C32 H60 O9	987	
		C29 H54 O7	987	

Name	CAS	Formula	Similarity	Class
		C20 H42 O6	987	
		C26 H50 N3 O5	987	
		C28 H54 N3 O8	987	
		C31 H61 N5 O4	987	
		C43 H84 N3 O13	988	
		C26 H49 N2 O2	988	
		C28 H55 N5 O3	988	
		C37 H70 O11	989	
		C39 H85 N4 O12	989	
		C28 H54 N3 O6	989	
		C23 H42 N4 O	989	
		C22 H41 O6	989	
		C44 H87 N5 O11	989	
		C26 H51 N5 O2	989	
		C24 H50 O13	989	
		C22 H47 N O	989	
		C29 H54 O7	989	
		C18 H38 O10	990	
		C42 H81 N2 O9	990	
		C28 H58 O10	990	
		C46 H91 N5 O12	990	
		C33 H62 O9	990	
		C38 H73 N2 O9	990	
		C41 H80 N3 O14	991	
		C26 H54 O14	991	
		C34 H65 N2 O6	991	
		C41 H80 N3 O13	991	
		C28 H58 O7	992	
		C21 H38 N4 O7	992	
		C22 H46 O7	992	
		C26 H55 N O4	992	
		C24 H50 O8	993	
		C26 H54 O9	993	
		C18 H38 O5	993	

Name	CAS	Formula	Similarity	Class
		C37 H73 N5 O7	993	
		C35 H66 O10	993	
		C12 H22 N3 O4	993	
		C50 H100 N2 O3 S	993	
		C24 H51 N O3	993	
		C47 H90 O15	993	
		C21 H43 O11	993	
		C18 H38 O4	994	
		C8 H19 N O2	994	
		C55 H110 N2 O3 S	994	
		C26 H55 N O4	995	
		C9 H18 N2 O3	995	
		C43 H82 O13	996	
		C26 H50 N2 O8	996	
		C24 H47 N5 O	996	
		C22 H47 N O3	996	
		C24 H51 N O4	996	
		C43 H84 N3 O14	996	
		C20 H43 N O	996	
		C30 H55 N5 O5	997	
		C14 H29 N O	997	
		C22 H46 O6	997	
		C22 H45 N O3	998	
		C24 H51 N O4	998	
		C23 H48 N2 O	999	

Raw sludge GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ Adipates					
DEHP	117-81-7	C24 H38 O4	948	Phthalate	262
DINP	28553-12-0	C26 H42 O4	759	Phthalate	232
Dibutyl phthalate	84-74-2	C16 H22 O4	919	Phthalate	166
1,2-Benzenedicarboxylic acid, dicyclohexyl ester	84-61-7	C20 H26 O4	848	Phthalate	137
Diethyl Phthalate	84-66-2	C12 H14 O4	941	Phthalate	55
Benzyl butyl phthalate	85-68-7	C19 H20 O4	853	Phthalate	10
Diisooctyl adipate	1330-86-5	C22 H42 O4	711	Adipate	2,6
Organophosphates					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	875	OP	30
2-Ethylhexyl diphenyl phosphate	1241-94-7	C20 H27 O4 P	804	OP	11
Propylated triphenyl phosphate	28108-99-8	C21 H21 O4 P	797	OP	9,1
Triphenyl phosphate	115-86-6	C18 H15 O4 P	851	OP	5,3
Tributyl phosphate	126-73-8	C12 H27 O4 P	736	OP	1,8
Triisobutyl phosphate	126-73-8	C12 H27 O4 P	703	OP	1,7
Cresyl diphenylphosphate	26444-49-5	C19 H17 O4 P	708	OP	1,7
Other polymer components/additives					
Oleyl nitrile	112-91-4	C18 H33 N	913	Plasticizer, OLN	220
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	929	Benzothiazole	75
1,2-Ethanediol, dibenzoate	94-49-5	C16 H14 O4	812	Plastics additive, plasticizer (Benzoflex 988)	59
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	C16 H30 O4	875	Ester, platicizer	51
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	874	Antioxidant degr. Prod.; Keto-ester	50
Acetophenone	98-86-2	C8 H8 O	961	Ketone, aromatic	29
Benzothiazole	95-16-9	C7 H5 N S	904	Benzothiazole	21
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	891	Antioxidant	18
Benzenethiol, 3-methyl-		C7 H8 S	869	Thiol	13
2,3-Dimethylphenyl isocyanate	1591-99-7	C9 H9 N O	847	Isocyanate	9,5

Name	CAS	Formula	Similarity	Class	ng/sample
Tributyl acetylcitrate	77-90-7	C20 H34 O8	740	Plastics additive, plasticizer	9,0
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	833	Benzothiazole	8,3
2-(Methylthio)phenyl isothiocyanate	51333-75-6	C8 H7 N S2	877	Isocyanate	7,6
Decanenitrile	1975-78-6	C10 H19 N	882	Nitrile	7,0
1,3-Benzothiazole, 2-(3-methylbutoxy)-	0-00-0	C12 H15 N O S	585	Benzothiazole	6,8
Ethanone, 2,2-dimethoxy-1,2-diphenyl-	24650-42-8	C16 H16 O3	854	Plastics additive, UV photoinitiator	6,3
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	883	Plasticizer	6,3
Benzothiazole, 2-(2-hydroxyethylthio)-	4665-63-8	C9 H9 N O S2	705	Benzothiazole	5,0
à,à,à',à'-Tetramethyl-1,4-benzenedimethanol	2948-46-1	C12 H18 O2	707	Bisphenol A	4,3
Triacetin	102-76-1	C9 H14 O6	782	Plastizicer, solvent, PPCP, E1518	2,3
Butylated Hydroxytoluene	128-37-0	C15 H24 O	768	Antioxidant	2,2
PPCP + flavour/fragrances					
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	5466-77-3	C18 H26 O3	907	PPCP, sunscreen (Escalol 557)	324
Galoxolide	1222-05-5	C18 H26 O	778	Musk	214
2-Pentadecanone, 6,10,14-trimethyl-	502-69-2	C18 H36 O	867	Artificial flavour?	60
Tonalid	21145-77-7	C18 H26 O	706	Musk	59
Delta-Tetradecalactone	92446-06-5	C14 H26 O2	859	Artificial flavour, "butter/cream flavour"	56
Benzophenone	119-61-9	C13 H10 O	927	PPCP	29
N,N-Dimethyldodecanamide	3007-53-2	C14 H29 N O	818	PPCP, surfactant	33
Delta-Tridecalactone	7370-92-5	C13 H24 O2	829	Artificial flavour, "butter/cream flavour"	16
2-Decanone	693-54-9	C10 H20 O	842	Artificial flavour, "orange flavour"	15
Gamma-Decalactone	706-14-9	C10 H18 O2	898	Artificial flavour, "peach/apricot flavour"	15
Gamma-Heptalactone	105-21-5	C7 H12 O2	879	Artificial flavour, "butter/cream flavour"	13
Homosalate	118-56-9	C16 H22 O3	777	PPCP, sunscreen	9,2
Delta-Decalactone	705-86-2	C10 H18 O2	798	Artificial flavour, "butter/cream flavour"	8,3
Cedrol	77-53-2	C15 H26 O	714	Terpenoid	7,9

Name	CAS	Formula	Similarity	Class	ng/sample
Gamma-Undecalactone	104-67-6	C11 H20 O2	874	Artificial flavour, "peach/apricot flavour"	6,1
5-Thiazoleethanol, 4-methyl-	137-00-8	C6 H9 N O S	881	Thiazole, hyroxy	5,8
Geranyl acetone	689-67-8	C14 H24 O	839	PPCP, fragrance (BASF)	4,4
Ar-tumerone	532-65-0	C15 H20 O	749	Pharma and phytochemical	4,0
á-Ionone epoxide	23267-57-4	C13 H20 O2	823	PPCP, fragrance	3,2
Benzyl Benzoate	120-51-4	C14 H12 O2	810	PPCP, plasticizer	1,8
gamma-Ionone	79-76-5	C13 H20 O	799	PPCP, fragrance	1,8
Lauryl acetate	57472-68-1	C14 H28 O2	863	PPCP	1,3
Halogenated compounds/ Pesticides					
Acetamide, 2-chloro-N-phenethyl-	13156-95-1	C10 H12Cl N O	924	Halogenated compound	29
Permethrin	52645-53-1	C21 H20Cl2 O3	753	Pesticide	8,9
Benzoic acid, 2,4-dichloro-	50-84-0	C7 H4Cl2 O2	812	Halogenated compound	6,8
Benzenamine, 2,4-dichloro-	554-00-7	C6 H5Cl2 N	702	Halogenated compound	3,8
m-Chloroaniline	108-42-9	C6 H6Cl N	749	Amine	2,4
Benzenecarbothioic acid, 2,6-dichloro-, S-methyl ester	68504-39-2	C8 H6Cl2 O S	778	Halogenated compound	1,6
1,1'-Biphenyl, 4,4'-dichloro-		C12 H8Cl2	708	PCB	1,4
Glycols					
Ethanol, 2-(dodecyloxy)-	4536-30-5	C14 H30 O2	785	Glycole	75
Ethanol, 2-(hexadecyloxy)-		C18 H38 O2	821	Glycole	19
Alkyl-benzenes					
Benzene, (1-methyldodecyl)-	4534-53-6	C19 H32	769	Alkylbenzene, branched (BAB)	141
Benzene, (1-butyloctyl)-	2719-63-3	C18 H30	865	Alkylbenzene, branched (BAB)	66
Benzene, (1-ethyldecyl)-	2400-00-2	C18 H30	838	Alkylbenzene, branched (BAB)	45
Benzene, (1-pentyloctyl)-	4534-49-0	C17 H28	809	Alkylbenzene, branched (BAB)	23
Benzene, 1-nonenyl-	34426-61-4	C15 H22	776	Alkylbenzene, branched (BAB)	20
Benzene, (1-butylheptyl)-	4537-15-9	C17 H28	888	Alkylbenzene, branched (BAB)	11
Benzene, (1-methyldecyl)-	4536-88-3	C17 H28	864	Alkylbenzene, branched (BAB)	10
Benzene, (1-butylnonyl)-	4534-50-3	C19 H32	785	Alkylbenzene, branched (BAB)	9,2
Benzene, (1-pentyloctyl)-	4534-49-0	C19 H32	743	Alkylbenzene, branched (BAB)	8,4
Benzene, (1-ethylnonyl)-	4536-87-2	C17 H28	821	Alkylbenzene, branched (BAB)	6,5
Benzene, 1-butenyl-, (E)-	1005-64-7	C10 H12	740	Alkylbenzene, branched (BAB)	5,8
Benzene, (1-propyloctyl)-	4536-86-1	C17 H28	855	Alkylbenzene, branched (BAB)	5,6

Name	CAS	Formula	Similarity	Class	ng/sample
Benzene, (1-propylnonyl)-	2719-64-4	C18 H30	860	Alkylbenzene, branched (BAB)	5,6
Benzene, (1-propyldecyl)-	4534-51-4	C19 H32	857	Alkylbenzene, branched (BAB)	5,3
Benzene, (1-methylundecyl)-	2719-61-1	C18 H30	835	Alkylbenzene, branched (BAB)	3,4
Benzene, pentyl-	538-68-1	C11 H16	845	Alkylbenzene, branched (BAB)	3,3
Benzene, hexyl-	1077-16-3	C12 H18	806	Alkylbenzene, branched (BAB)	2,5
Benzene, butyl-	104-51-8	C10 H14	757	Alkylbenzene, branched (BAB)	2,2
Benzene, (1-methylnonyl)-	4537-13-7	C16 H26	791	Alkylbenzene, branched (BAB)	1,9
Benzene, (1-ethyloctyl)-	4621-36-7	C16 H26	743	Alkylbenzene, branched (BAB)	0,9
Hex-1-enylbenzene	828-15-9	C12 H16	757	Alkylbenzene, branched (BAB)	0,1
Benzoic acid esters					
Benzoic acid, pentadecyl ester		C22 H36 O2	838	Benzoic acid ester	22
Benzoic acid, tridecyl ester		C20 H32 O5	822	Benzoic acid ester	18
Benzoic acid, 2-ethylhexyl ester	5444-75-7	C15 H22 O2	826	Benzoic acid ester	8,1
Benzoic acid, tetradecyl ester		C21 H34 O2	868	Benzoic acid ester	5,7
Various amides/amines					
Ethanone, 1-(2-aminophenyl)-	551-93-9	C8 H9 N O	943	Amine, Ketone, aromatic	57
Acetamide, N-(2-phenylethyl)-	877-95-2	C10 H13 N O	904	Amide, aromatic	7,0
Benzeneacetamide, N,N-dimethyl-	18925-69-4	C10 H13 N O	881	Amide, aromatic	6,7
Morpholine, 4-(phenylacetyl)-	17123-83-0	C12 H15 N O2	779	Amide, aromatic	1,0
N-(1-Cyano-1-methylethyl)isobutyramide	84213-57-0	C8 H14 N2 O	768	Amide, Cyano	2,9
3-Acetamidoacetophenone	7463-31-2	C10 H11 N O2	798	Amide, Ketone, aromatic	2,5
Formamide, (2-acetylphenyl)-	0-00-0	C9 H9 N O2	766	Amide, Ketone, aromatic	0,6
Various ketones, esters, aldehydes					
6-Methyl-2-pyridinecarbaldehyde	53547-60-7	C7 H7 N O	817	N-hetrocyclic, Aldehyde	9,7
Ethanone, 1,1'-(1,3-phenylene)bis-	6781-42-6	C10 H10 O2	843	Ketone, aromatic	7,4
Formic acid, 2-phenylethyl ester	104-62-1	C9 H10 O2	876	Aldehyde, aromatic	6,4
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	C13 H22 O3	781	Keto-ester	6,4
Cyclohexyl-á-phenylpropionate	22847-18-3	C15 H20 O2	756	Ester, aromatic	2,6
2-Butanone, 4-(5-methyl-2-furanyl)-	13679-56-6	C9 H12 O2	750	Keto-ether	1,7
PAC					
Fluoranthene	129-00-0	C16 H10	787	PAH	207
Benzo[k]fluoranthene		C20 H12	902	PAH	74

Name	CAS	Formula	Similarity	Class	ng/sample
Benzo[k]fluoranthene	207-08-9	C20 H12	875	PAH	71
Phenanthrene, 2,3,5-trimethyl-		C17 H16	836	Alkyl-PAH	60
Phenanthrene, 2,3-dimethyl-		C16 H14	885	Alkyl-PAH	41
9H-Fluorene, 2,3-dimethyl-	4612-63-9	C15 H14	845	O-PAH	37
Phenanthrene, 1,7-dimethyl-		C16 H14	879	Alkyl-PAH	35
Phenanthrene, 2,3,5-trimethyl-		C17 H16	835	Alkyl-PAH	34
Benzo[b]naphtho[1,2-d]furan	239-30-5	C16 H10 O	701	O-PAH	31
9-Fluorenone, 2.4-dimethyl-		C16 H14	787	Alkyl-PAH	26
Phenanthrene, 3,6-dimethyl-		C16 H14	850	Alkyl-PAH	26
Naphthalene, 1-(phenylmethoxy)-	607-58-9	C17 H14 O	817	O-PAH	24
Dibenzofuran, 4-methyl-		C13 H10 O	790	O-PAH	24
Naphtho[2,1-b]furan, 1,2-dimethyl-	129812-23-3	C14 H12 O	794	O-PAH	23
Pyrene	129-00-0	C16 H10	892	PAH	22
Phenanthrene, 1-methyl-		C15 H12	891	Alkyl-PAH	22
Pyrene, 4-methyl-		C17 H12	792	Alkyl-PAH	20
Benzo[k]fluoranthene		C20 H12	714	PAH	20
Phenanthrene	85-01-8	C14 H10	951	PAH	19
1,4,5,8-Tetramethylnaphthalene		C14 H16	783	Alkyl-PAH	19
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	797	Alkyl-PAH	18
Benzo[k]fluoranthene		C20 H12	879	PAH	18
Naphthalene, 1-methyl-7-(1-methylethyl)-		C14 H16	849	Alkyl-PAH	17
Anthracene, 1-methyl-		C15 H12	914	Alkyl-PAH	16
Anthracene, 1,2,3,4-tetrahydro-	2141-42-6	C14 H14	876	PAH	16
Benzo[k]fluoranthene	207-08-9	C20 H12	706	PAH	16
Azulene, 7-ethyl-1,4-dimethyl-		C14 H16	886	Alkyl-PAH	15
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl-		C18 H20	867	Alkyl-PAH	15
2,6-Diisopropylnaphthalene	24157-81-1	C16 H20	771	Alkyl-PAH	14
Naphthalene, 1,4,5-trimethyl-		C20 H12	895	Alkyl-PAH	14
Naphthalene, 1,4,6-trimethyl-		C20 H12	916	Alkyl-PAH	14
Naphthalene, 1,4,5-trimethyl-		C20 H12	893	Alkyl-PAH	14
Naphthalene, 1-methyl-7-(1-methylethyl)-		C14 H16	757	Alkyl-PAH	13
1,1'-Biphenyl, 2-ethyl-		C14 H14	840	Alkyl-PAH	11
9H-Fluorene, 2-methyl-		C14 H12	829	Alkyl-PAH	10
11H-Benzo[b]fluorene	243-17-4	C17 H12	771	PAH	10
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	823	Alkyl-PAH	10
Naphthalene, 1,2,3,4-tetramethyl-		C14 H16	811	Alkyl-PAH	10

Name	CAS	Formula	Similarity	Class	ng/sample
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	814	Alkyl-PAH	10
Phenanthrene, 3,4,5,6-tetramethyl-		C18 H18	738	Alkyl-PAH	10
Benzene, 1,2-dimethyl-4-(phenylmethyl)-		C15 H16	823	Alkyl-PAH	9,8
Phenanthrene, 1-methyl-		C15 H12	817	Alkyl-PAH	9,7
Pyrene, 4-methyl-		C17 H12	788	Alkyl-PAH	9,3
6H-Dibenzo[b,d]-pyran	229-95-8	C13 H10 O	791	O-PAH	8,8
Benzo[k]fluoranthene		C20 H12	704	PAH	8,7
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	798	Alkyl-PAH	8,5
3-Phenyl-benzofuran	29909-72-6	C14 H10 O	866	PAH	8,0
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	899	Alkyl-PAH	7,8
2,6-Diisopropylnaphthalene		C16 H20	808	Alkyl-PAH	7,6
Benzenemethanol, à-phenyl-	91-01-0	C13 H12 O	752	O-PAH	7,5
4-Quinolinol, 2-methyl-	607-67-0	C10 H9 N O	770	N-heterocyclic	7,5
Diphenylmethoxy acetic acid	21409-25-6	C15 H14 O3	762	O-PAH	6,6
Naphthalene, 1,2,3,4-tetramethyl-		C14 H16	835	Alkyl-PAH	6,6
Naphthalene, 2-methyl-1-propyl-		C20 H12	865	Alkyl-PAH	6,5
Naphthalene, 2-methyl-1-propyl-		C20 H12	763	Alkyl-PAH	6,2
8-Quinolinol, 7-methyl-	5541-68-4	C10 H9 N O	881	N-heterocyclic	5,7
Naphthalene, 1-methyl-7-(1-methylethyl)-		C14 H16	790	Alkyl-PAH	5,6
Benz[a]anthracene	56-55-3	C18 H12	903	PAH	5,5
Naphthalene, 1,4,5-trimethyl-		C20 H12	795	Alkyl-PAH	5,4
1,1'-Biphenyl, 2-ethyl-		C14 H14	841	Alkyl-PAH	5,2
Ethanedione, diphenyl-	134-81-6	C14 H10 O2	924	O-PAH	5,2
Benz[a]anthracene	56-55-3	C18 H12	700	PAH	5,1
2,8-Dimethyldibenzo(b,d)thiophene	1207-15-4	C14 H12 S	794	S-PAH	5,0
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	892	Alkyl-PAH	4,5
Dibenzofuran, 4-methyl-		C13 H10 O	830	O-PAH	4,4
Naphthalene, 2-(1-methylethyl)-		C13 H14	856	Alkyl-PAH	4,4
Phenanthrene, 4,5-dimethyl-		C16 H14	779	Alkyl-PAH	4,3
Fluorene	86-73-7	C13 H10	891	PAH	3,9
Dibenzothiophene, 4-methyl-		C13 H10 S	856	S-PAH	3,8
Naphthalene, 2,3-dimethyl-		C12 H12	804	Alkyl-PAH	3,8
Naphthalene, 1-methyl-7-(1-methylethyl)-		C14 H16	826	Alkyl-PAH	3,7
Naphthalene, 2-methyl-1-propyl-	54774-89-9	C20 H12	767	Alkyl-PAH	3,5
Anthracene, 9,10-dihydro-2-methyl-	948-67-4	C15 H14	778	Alkyl-PAH	3,4
2,6-Diisopropylnaphthalene		C16 H20	808	Alkyl-PAH	3,3

Name	CAS	Formula	Similarity	Class	ng/sample
Naphthalene, 2-(1-methylethyl)-		C13 H14	819	Alkyl-PAH	3,3
9H-Fluorene, 1-methyl-		C14 H12	905	Alkyl-PAH	3,3
2-Phenylnaphthalene	35465-71-5	C16 H12	826	PAH	3,2
1,1'-Biphenyl, 4-methyl-		C13 H12	871	Alkyl-PAH	3,1
1,1'-Biphenyl, 4-methyl-		C13 H12	901	Alkyl-PAH	2,9
Naphthalene, 1-methyl-7-(1-methylethyl)-	490-65-3	C14 H16	801	Alkyl-PAH	2,8
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	13540-56-2	C15 H16	816	Alkyl-PAH	2,8
Piperonal	120-57-0	C8 H6 O3	811	O-PAH	2,6
Thiophene, 2-(3-methylbutyl)-	26963-33-7	C9 H14 S	858	S-PAH	1,9
Indole-5-aldehyde	1196-69-6	C9 H7 N O	817	N-heterocyclic, aldehyde	1,9
9H-Fluorene, 1-methyl-		C14 H12	905	Alkyl-PAH	1,7
2,6-Diisopropylnaphthalene		C16 H20	808	Alkyl-PAH	1,6
Benzo[a]pyrene	50-32-8	C20 H12	749	PAH	1,6
Naphtho[2,1-b]thiophene	233-02-3	C12 H8 S	783	S-PAH	1,4
Naphthalene, 1,7-dimethyl-		C12 H12	771	Alkyl-PAH	1,2
Benzo[e]pyrene		C20 H12	753	PAH	1,2
Anthracene, 9-ethenyl-		C16 H20	843	Alkyl-PAH	0,8
Benzo[h]cinnoline	230-31-9	C12 H8 N2	735	N-PAH	0,5
11H-Benzo[a]fluoren-11-one	479-79-8	C17 H10 O	743	O-PAH	0,4
Indene	95-13-6	C9 H8	770	PAH	0,1

Raw sludge LC-MS

Name	CAS	Formula	Similarity	Class
Phthalates				
DEHP		C24 H38 O4	843	Phthalate
Biocides				
Domiodol	61869-07-6	C5 H9 I O3	734	Molluscicide
Mepanipyrim		C14 H13 N3	725	Fungicide
Mipafox	371-86-8	C6 H16 F N2 O P	748	Insecticide
Pharmaceuticals				
Niclofolan	10331-57-4	C12 H6 Cl2 N2 O6	707	Anthelmintic
Spirapril hydrochloride		C22H30N2O5S2	903	ACE inhibitor antihypertensive drug used to treat hypertension.
Not identified				
		C42 H63 N2 O3	646	
		C15 H8 N3 O3	662	
		C12 H N O10	663	
		C19 H41 Cl N O6	663	
		C11 H4 N2 O2	668	
		C18 H27 O	668	
		C31 H46 N O	670	
		C30 H53 Cl N O2	671	
		C50 H98 Cl N O10	672	
		C13 H28 N2 O4	680	
		C20 H26 Cl N2 O2	680	
		C39 H65 N2 O	680	
		C24 H32 N O	687	
		C40 H62 O4	688	
		C33 H64 Cl N2 O9	693	
		C30 H44 N O	696	
		C47 H64 Cl O2	698	
		C40 H63 N2 O2	708	
		C15 H4 N O2	710	

Name	CAS	Formula	Similarity	Class
		C18 H27 O	713	
		C45 H82 O6	721	
		C52 H73 Cl N2 O2	721	
		C46 H62 Cl O2	722	
		C39 H60 O4	723	
		C11 H19 N3 O2	732	
		C32 H48 N O	733	
		C52 H103 N O6	734	
		C33 H64 Cl N2 O9	735	
		C31 H62 N O9	738	
		C41 H70 Cl O2	746	
		C30 H44 N O	748	
		C35 H61 O6	750	
		C42 H63 N2 O2	763	
		C17 H12 O	763	
		C38 H58 N O3	766	
		C45 H62 Cl N3 O	766	
		C30 H54 N3 O4	771	
		C33 H50 N O	774	
		C36 H71 Br N O5	775	
		C19 H35 Br O4	776	
		C50 H88 N3 O7	777	
		C29 H58 N O8	786	
		C40 H77 N O12	790	
		C4 H5 Cl3 N2 O2	790	
		C24 H25 Cl N2 O12	796	
		C59 H94 Cl2 N3 O	799	
		C4 H5 Cl3 N2 O2	802	
		C40 H77 N O12	810	
		C24 H32 N O	811	
		C40 H75 N O11	813	
		C39 H58 O3	819	
		C40 H63 N2 O3	822	
		C36 H70 Cl N2 O4	833	

Name	CAS	Formula	Similarity	Class
		C21 H27 Br Cl N2 O3	839	
		C51 H67 N3 O	840	
		C38 H64 Cl2 N2 O2	843	
		C4 H5 Cl3 N2 O2	843	
		C8 H4 Br Cl N O7	843	
		C20 H30 Br Cl N O	852	
		C21 H27 Br Cl N2 O3	859	
		C38 H64 N3 O3	861	
		C16 H33 Br O2	862	
		C31 H62 N O9	869	
		C34 H68 N2 O14	876	
		C19 H N2 O8	883	
		C28 H52 O7	902	
		C52 H101 N O5	905	
		C20 H27 Br Cl2 N O3	911	
		C51 H103 N O6	911	
		C44 H80 N O14	913	
		C31 H58 Cl2 N O10	913	
		C25 H32 Cl4 O4	915	
		C45 H61 N3 O	916	
		C22 H22 Br N O4	922	
		C6 H Br Cl2 N O5	923	
		C6 H Br Cl2 N O5	926	
		C6 H Br Cl2 N O5	927	
		C42 H84 O5	938	
		C18 H22 Br Cl5 N3 O	951	
		C52 H97 Cl3 O9	953	
		C30 H60 N2 O8	963	
		C36 H68 O4	969	
		C30 H54 O7	977	

Influent GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ Adipates					
Dibutyl phthalate	84-74-2	C16 H22 O4	937	Phthalate	119
Diisobutyl phthalate	84-69-5	C16 H22 O4	891	Phthalate	50
Diethyl Phthalate	84-66-2	C12 H14 O4	945	Phthalate	39
DEHP	117-81-7	C24 H38 O4	935	Phthalate	31
Benzyl butyl phthalate	85-68-7	C19 H20 O4	798	Phthalate	5,5
Dimethyl phthalate	131-11-3	C10 H10 O4	721	Phthalate	4,8
Organophosphates					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	902	OP	38
Ethanol, 2-butoxy-, phosphate (3:1)	78-51-3	C18 H39 O7 P	762	OP	11
Triphenyl phosphate	115-86-6	C18 H15 O4 P	567	OP	2,5
Tributyl phosphate	126-73-8	C12 H27 O4 P	759	OP	1,7
Tri(2-chloroethyl) phosphate	115-96-8	C6 H12Cl3 O4 P	727	OP	1,0
Other polymer components/additives					
Oleyl nitrile	112-91-4	C18 H33 N	913	Plasticizer, OLN	289
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	942	Benzothiazole	202
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	895	Antioxidant	43
11-Octadecynenitrile		C18 H31 N	794	Nitrile	41
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	881	Antioxidant degr. Prod.; Keto-ester	32
Benzothiazole, 2-(methylthio)-	615-22-5	C8 H7 N S2	889	Benzothiazole	30
Benzothiazole	95-16-9	C7 H5 N S	894	Benzothiazole	17
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	778	Benzothiazole	16
Disulfide, bis(4-methylphenyl)	103-19-5	C14 H14 S2	838	Disulfide, cross linking agent	15
Ethanedione, diphenyl-	134-81-6	C14 H10 O2	867	Photoinitiator (benzil)	13
2,4,7,9-Tetramethyl-5-decyn-4,7-diol	126-86-3	C14 H26 O2	816	Defoamer (BASF)	13
Acetophenone	98-86-2	C8 H8 O	822	Ketone, aromatic	13
Benzenesulfonamide, 4-methyl-	70-55-3	C7 H9 N O2 S	708	Plasticizer	11
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-	74381-40-1	C16 H30 O4	854	Ester, platicizer	9,9

Name	CAS	Formula	Similarity	Class	ng/sample
propanediyl ester					
1-Ethyl-2-pyrrolidinone	2687-91-4	C6 H11 N O	835	Solvent	9,8
Triacetin	102-76-1	C9 H14 O6	900	Plastizicer, solvent, PPCP, E1518	8,9
Ethanone, 2,2-dimethoxy-1,2-diphenyl-	24650-42-8	C16 H16 O3	841	Plastics additive, UV photoinitiator	8,5
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	884	Plasticizer	7,9
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	C15 H22 O2	827	Antioxidant	7,3
Bernzothiazole, 2-[2-(2-fluorophenoxy)ethylthio]-	330955-62-9	C15 H12F N O S2	727	Benzothiazole	7,3
2-Benzothiazolamine, N-ethyl-	28291-69-2	C9 H10 N2 S	779	Benzothiazole	5,7
Tributyl acetylcitrate	77-90-7	C20 H34 O8	829	Plasticiser, antifoaming agent	5,5
Benzenesulfonamide, N-phenyl-	1678-25-7	C12 H11 N O2 S	701	Plasticizer	3,9
Benzenesulfonamide, N-ethyl-2-methyl-	1077-56-1	C9 H13 N O2 S	689	Plasticizer	3,6
Tetradecanenitrile		C14 H27 N	760	Nitrile	3,5
3,5-di-tert-Butyl-4-hydroxyacetophenone	14035-33-7	C16 H24 O2	827	Antioxidant	3,3
Benzoic acid, 2-benzoyl-, methyl ester	606-28-0	C15 H12 O3	806	Photoinitiator (MBB)	2,7
Phenol, 2,4-di-t-butyl-6-nitro-	20039-94-5	C14 H21 N O3	758	Antioxidant	2,1
Benzothiazole, 2-(2-hydroxyethylthio)-	4665-63-8	C9 H9 N O S2	708	Benzothiazole	1,9
2,3-Dimethylphenyl isocyanate	1591-99-7	C9 H9 N O	742	Isocyanate	1,3
Butylated Hydroxytoluene	128-37-0	C15 H24 O	722	Antioxidant	0,9
Bayer 28,589	728-40-5	C14 H21 N O3	712	Antioxidant	0,3
PPCP + flavour/fragrances					
N,N,N',N'-Tetraacetylethylenediamine (TAED)	10543-57-4	C10 H16 N2 O4	920	Peroxide bleach activator	90
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	C13 H22 O3	812	Perfume (hedione) "jasmin aroma", isomer	37
Benzhydrol	91-01-0	C13 H12 O	867	Perfume fixative...	34
2-Dodecanol	10203-28-8	C12 H26 O	772	Surfactant, solvent	31
ç Dodecalactone	2305-05-7	C12 H22 O2	865	Artificial flavour, "peach/apricot flavour"	27
N,N-Dimethyldodecanamide	3007-53-2	C14 H29 N O	879	Surfactant, solvent	18
epsilon-Dodecalactone	16429-21-3	C12 H22 O2	873	Artificial flavour, "fruity"	15
Benzophenone	119-61-9	C13 H10 O	818	UV-blocker	14
Caffeine	58-08-2	C8 H10 N4 O2	897	Food ingredient	14
N,N-Dimethyldecanamide	14433-76-2	C12 H25 N O	793	Surfactant, solvent	13

Name	CAS	Formula	Similarity	Class	ng/sample
Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester	74367-33-2	C12 H24 O3	767	Perfume (hedione) "jasmin aroma", isomer	11
Gamma-Undecalactone	104-67-6	C11 H20 O2	813	Artificial flavour, "peach/apricot flavour"	11
Gamma-Decalactone	706-14-9	C10 H18 O2	887	Artificial flavour, "peach/apricot flavour"	8,8
Acetamide, N-acetyl-N,N'-1,2-ethanediylbis-	137706-80-0	C8 H14 N2 O3	765	TAED - acetyl	1,8
Crotamiton	483-63-6	C13 H17 N O	779	Pharmaceutical	0,7
Halogenated compounds/ Pesticides					
Benzamide, N,N-diethyl-3-methyl- (DEET)	2728-05-4	C12 H17 N O	869	Pesticide	6,6
Glycols					
Diethylene glycol monododecyl ether	3055-93-4	C16 H34 O3	781	Glycole	36
1-Propanol, 2,2'-oxybis-	108-61-2	C6 H14 O3	834	Glycole	21
2-Propenoic acid, (1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] ester		C15 H24 O6	786	Glycole	12
Ethanol, 2-(2-butoxyethoxy)-, acetate		C10 H20 O4	891	Glycole	8,6
2-Propanol, 1-[2-(2-methoxy-1-methylethoxy)-1-methylethoxy]-	20324-33-8	C10 H22 O4	755	Glycole	6,6
Ethanol, 2-(dodecyloxy)-		C14 H30 O2	762	Glycole	5,9
Various N-compounds					
1H-Imidazole, 1-methyl-5-nitro-	3034-42-2	C4 H5 N3 O2	755	N-hererocycle	23
Various ketones, esters, aldehydes					
Ethanone, 1,1'-(1,3-phenylene)bis-	6781-42-6	C10 H10 O2	826	Ester, aromatic	18
Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	C12 H24 O3	780	Ester, hydroxy-	14
Ethanone, 1,1'-(1,4-phenylene)bis-	1009-61-6	C10 H10 O2	772	Ester, aromatic	4,7
Alkyl-benzenes					
Benzene, (1-butyloctyl)-		C18 H30	818	Benzene, alkyl-	3,5
PAC					

Name	CAS	Formula	Similarity	Class	ng/sample
2H-Indol-2-one, 1,3-dihydro-	59-48-3	C8 H7 N O	914	O-PAC	14
Phenanthrene	85-01-8	C14 H10	764	PAH	6,4
2,6-Diisopropylnaphthalene		C16 H20	779	Alkyl-PAH	3,9
2H-1-Benzopyran-2-one	91-64-5	C9 H6 O2	706	O-PAC	3,0
Fluorene	86-73-7	C13 H10	764	PAH	1,2
Pyrene	129-00-0	C16 H10	701	PAH	0,7
1(3H)-Isobenzofuranone	87-41-2	C8 H6 O2	756	O-PAC	0,7
2,6-Diisopropylnaphthalene		C16 H20	811	Alkyl-PAH	0,3
2,6-Diisopropylnaphthalene		C16 H20	764	Alkyl-PAH	0,2

Influent LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Neoquassin	76-77-7	C22 H30 O6	900	biocide
PFCs				
PFHxA		C6 H F11 O2	655	PFCs
PFNA		C9 H F17 O2	669	PFCs
PFOS		C8 H F17 O3 S	676	PFCs
Phthalates				
benzyl butyl phthalate		C19 H20 O4	671	phthalate
OPs				
Ethanol, 2-butoxy-, phosphate (3:1)		C18 H39 O7 P	725	OP
Tri(2-chloroethyl) phosphate		C6 H12 Cl3 O4 P	649	OP
UV absorbers				
UV-234		C30 H29 N3 O	738	benzotriazole
UV-327		C20 H24 Cl N3 O	663	benzotriazole
UV-329		C20 H25 N3 O	887	benzotriazole
Additives				
dicyclohexylamine (DCHA)		C12 H23 N	837	benzenediamine
Benzenesulfonamide, N-butyl-		C10 H15 N O2 S	661	Plasticizer
Pharmaceuticals and biomolecules				
2-propyl-tridecanoic acid		C16 H32 O2	995	
Argatroban	74863-84-6	C23 H36 N6 O5 S	696	Hemostatic
Buspirone	36505-84-7	C21 H31 N5 O2	941	Tranquilizer
Caffeine		C8 H10 N4 O2	780	
Cannabidiolic acid		C22 H30 O4	442	
Carebastine	90729-42-3	C32 H37 N O4	879	Antihistamine
Despropionylbezitramide	83898-28-6	C28 H28 N4 O	765	bezitramide metabolite
Ditazol	18471-20-0	C19 H20 N2 O3	775	Thromb.Aggr. Inihib.
Eplerenone	107724-20-9	C24 H30 O6	919	antihypertensive
Ethyldibunate	5560-69-0	C20 H28 O3 S	863	Antitussive
Fexofenadine	83799-24-0	C32 H39 N O4	757	antihistaminic

Name	CAS	Formula	Similarity	Class
Homoprenorphine	16549-56-7	C28 H37 N O4	870	Analgesic
Laberalol		C19 H24 N2 O3	823	
Morin		C15 H10 O7	686	
N-Tris[hydroxymethyl]methyl-2-aminoethanesulfonic acid [TES]	7365-44-8	C6 H15 N O6 S	689	
Phenazone artifact	1251-85-0	C23 H24 N4 O2	825	Analgesic
Strophanthin, G	630-60-4	C29 H44 O12	785	Cardiotonic
Tioperidone	52618-67-4	C25 H32 N4 O2 S	829	Neuroleptic
Tixocortol	61951-99-3	C21 H30 O4 S	861	Corticoid
Tocamphyl	465-27-0	C19 H26 O4	960	
		C14 H33 N7 O6 S	655	
		C17 H35 N9 O8	657	
		C30 H47 N3 O9	741	
		C30 H43 N3 O8	746	
		C30 H43 N3 O8	751	
		C17 H45 N9 O11	752	
		C19 H31 N23 O	755	
		C12 H22 N6 O6	760	
		C17 H41 N11 O10	760	
		C22 H39 N13 O9	764	
		C13 H27 N9 O6	766	
		C17 H33 N13 O6	772	
		C26 H51 N7 O9	774	
		C24 H47 N17 O3	774	
		C21 H37 N17 O3	775	
		C28 H41 N3 O6	781	
		C18 H43 N13 O7	782	
		C18 H45 N13 O8	783	
		C18 H41 N13 O6	784	
		C27 H39 N7 O2	786	
		C25 H35 N13	787	
		C18 H31 N17 O3	788	
		C10 H25 N7 O4 S	802	
		C18 H33 N17 O3	815	

Name	CAS	Formula	Similarity	Class
		C23 H35 N17 O	816	
		C17 H26 N20	818	
		C20 H30 O6	819	
		C20 H34 N10 O6	819	
		C19 H31 N23	821	
		C13 H16 N10 O4	825	
		C18 H30 N10 O5	825	
		C16 H26 N10 O4	829	
		C17 H29 N5 O7	831	
		C17 H26 N10 O3	835	
		C9 H18 N6 O5	837	
		C15 H20 N10 O5	837	
		C27 H48 N2 O10	838	
		C26 H55 N3 O3 S3	842	
		C23 H51 N9 S4	843	
		C21 H26 N4 O2	845	
		C26 H46 Cl N9 S	849	
		C16 H32 N6 O6	849	
		C9 H19 N9 O4	850	
		C14 H27 N O7 S	851	
		C11 H23 N9 O5	856	
		C17 H35 N O2	860	
		C17 H24 O4	860	
		C15 H31 N9 O7	863	
		C22 H42 N16 O2 S2	870	
		C7 H16 O3	871	
		C20 H44 N4 O11	871	
		C16 H30 N6 O9	877	
		C15 H37 N11 O9	878	
		C21 H45 N13 O S2	879	
		C25 H49 N3 O8 S	889	
		C17 H26 O10	890	
		C18 H39 N O11	894	
		C23 H43 N9 O13	895	

Name	CAS	Formula	Similarity	Class
		C25 H47 N7 O4 S2	898	
		C19 H32 N8 O14	898	
		C25 H51 N3 O8 S	899	
		C26 H49 N7 O4 S	899	
		C6 H10 N6 O4	901	
		C10 H12 N10 O	904	
		C20 H43 N13 O7	905	
		C13 H18 O8	906	
		C18 H37 N19 O5	906	
		C24 H44 O15 S	910	
		C11 H18 N6 O7	912	
		C16 H32 O10	918	
		C18 H24 N12 O9	922	
		C8 H16 N10	922	
		C18 H45 N13 O8	925	
		C19 H45 N9 O11	926	
		C25 H51 N3 O8 S	926	
		C10 H12 N10 O	927	
		C21 H39 N17 O3	928	
		C19 H50 N12 O12 S	928	
		C26 H40 N8	930	
		C33 H47 N O5	930	
		C20 H45 N7 O7	930	
		C34 H45 N3 O7	930	
		C26 H48 O16 S	931	
		C15 H24 N10 O4	932	
		C30 H39 N11	933	
		C25 H49 N3 O15	934	
		C11 H16 O6	935	
		C20 H39 N13 S	935	
		C8 H14 N6 O5	936	
		C12 H16 N10 O2	936	
		C15 H37 N13 O7	936	
		C15 H37 N13 O7	936	

Name	CAS	Formula	Similarity	Class
		C20 H39 N13 O5	937	
		C31 H45 N O4	937	
		C27 H39 N7 O2	938	
		C27 H47 N3 O6 S	939	
		C29 H43 N7 O4	940	
		C23 H47 N5 S	941	
		C29 H43 N7 O3	943	
		C29 H43 N7 O4	944	
		C29 H49 N3 O6 S	945	
		C17 H37 N17 O	947	
		C17 H34 N6 O8	947	
		C26 H37 N7 O3	948	
		C10 H18 N6 O5	948	
		C17 H24 N10 O6	948	
		C19 H30 O11	948	
		C28 H45 N3 O6	950	
		C24 H41 N13 O2 S	950	
		C21 H37 N17 O	950	
		C17 H34 N6 O9	950	
		C19 H39 N17 O	950	
		C25 H37 N13	951	
		C19 H39 N17 O	951	
		C31 H41 N7 O2	952	
		C15 H30 N6 O8	953	
		C22 H43 N13 O S	953	
		C19 H39 N17 O	954	
		C24 H45 N15 O4	955	
		C22 H48 N12 O10 S	955	
		C20 H37 N19 O3	955	
		C10 H20 N6 O5	956	
		C10 H18 N6 O6	956	
		C18 H32 O12 S	956	
		C19 H36 N6 O10	957	
		C15 H37 N13 O7	957	

Name	CAS	Formula	Similarity	Class
		C18 H36 N6 O7	957	
		C26 H39 N7 O2	957	
		C14 H28 N6 O5	958	
		C7 H14 N6 O3	958	
		C14 H31 N O9	958	
		C24 H45 N7 O7	959	
		C27 H53 N7 O9	959	
		C17 H35 N O2	959	
		C19 H28 N10 O7	960	
		C25 H49 N3 O7 S	960	
		C26 H47 N7 O4 S	960	
		C25 H51 N3 O7 S	960	
		C11 H20 N6 O6	962	
		C19 H38 N6 O9	962	
		C24 H41 N3 O6	963	
		C18 H44 N16 O4 S	963	
		C28 H49 N O13	963	
		C20 H40 N6 O13 S	963	
		C32 H41 N O6	963	
		C12 H22 N6 O7	964	
		C14 H26 N6 O6	965	
		C20 H40 N6 O9 S	965	
		C22 H47 N O13	965	
		C16 H32 N6 O7 S	966	
		C22 H39 N13 S	967	
		C18 H33 N17 O3	968	
		C23 H40 N10 O5	968	
		C21 H36 N10 O4	970	
		C23 H49 N O13	970	
		C29 H57 N5 O11	971	
		C14 H26 N6 O8	971	
		C22 H41 N13 O7	973	
		C13 H20 N8 O11	973	
		C18 H36 N6 O12 S	973	

Name	CAS	Formula	Similarity	Class
		C15 H28 N6 O8	974	
		C13 H24 N6 O7	975	
		C22 H49 N7 O7	975	
		C15 H33 N O9	976	
		C28 H56 N6 O14	976	
		C16 H32 N6 O11 S	976	
		C20 H40 O12	977	
		C25 H50 N6 O12	977	
		C22 H41 N13 O5	977	
		C14 H28 N6 O7	979	
		C26 H45 N7 O9	979	
		C15 H30 N6 O7	980	
		C19 H41 N O11	980	
		C19 H40 O10	980	
		C21 H33 N5	981	
		C17 H37 N O2	982	
		C32 H47 N3 O6	982	
		C27 H53 N7 O9	982	
		C31 H61 N5 O12	983	
		C33 H60 N10 O12	983	
		C22 H43 N13 O2 S	984	
		C17 H32 N6 O9	984	
		C24 H45 N7 O11	984	
		C18 H34 N6 O10	984	
		C21 H32 N10 O8	985	
		C13 H24 N6 O7	985	
		C14 H30 O8	986	
		C17 H37 N O10	987	
		C19 H41 N O2	987	
		C27 H39 N3 O6	987	
		C17 H37 N7 O2	988	
		C18 H38 O10	988	
		C33 H65 N5 O13	988	
		C22 H49 N7 O7	988	

Name	CAS	Formula	Similarity	Class
		C17 H36 O9	989	
		C17 H32 N6 O9	989	
		C16 H35 N O2	989	
		C8 H18 O5	989	
		C20 H38 N6 O11	989	
		C21 H44 O11	989	
		C19 H41 N O3	990	
		C27 H43 N O4	991	
		C20 H42 O11	991	
		C25 H51 N7 O9	991	
		C24 H50 O13	993	
		C27 H53 N19 O4 S	993	
		C22 H45 N3 O8 S	993	
		C16 H34 O9	994	
		C7 H16 O3	995	
		C22 H46 O12	995	
		C10 H22 O6	995	
		C22 H49 N7 O7	995	
		C24 H49 N7 O9	995	
		C20 H42 O11	997	
		C11 H14 N3 O4	671	
		C7 H3 N4 O5	678	
		C11 H24 N O5	691	
		C7 H21 N4 O S	692	
		C6 H4 N6 O2 S	710	
		C22 H31 O	710	
		C7 H17 N3 O S	730	
		C7 H3 N2 O5 S	744	
		C8 H6 N3 O3 S	766	
		C11 H16 N5 O2	772	
		C3 H14 N7 O2	781	
		C5 H5 N2 O7	808	
		C5 H15 N5 O4	829	
		C6 H16 N O6	854	

Name	CAS	Formula	Similarity	Class
		C8 H6 O8	864	
		C7 H13 O8	726	
		C16 H23 N8	658	
		C8 H N2 O7	688	
		C10 H15 Cl3 N4	476	
		C7 H11 N4 O5	756	
		C7 H15 N7 O3 S	648	
		C9 H16 N3 O4 S	732	
		C7 H13 N5 O4	769	
		C16 H34 Cl2 N9 O2 S	479	
		C18 H30 N3 O	855	
		C22 H43 Cl N4 S	672	
		C25 H55 N27 O	646	
		C36 H75 N11 S4	356	
		C42 H67 N5 O4 S	954	
		C42 H62 N3	961	
		C46 H80 Cl O	734	
		C33 H71 N15 O S	952	
		C29 H63 Cl N15	987	
		C15 H35 Cl N6 O2	391	
		C42 H76 Cl O2	787	
		C13 H31 Cl N5 O3	425	
		C18 H39 N13 O7	358	
		C37 H78 Cl N3 O S	791	
		C27 H57 N24 O2	709	
		C43 H72 N2 O5 S2	615	
		C46 H76 N S	793	
		C27 H57 N26 O3	531	
		C27 H29 Cl N4 O2 S3	347	
		C29 H60 N12 O2	976	
		C33 H73 Cl2 N11 O4	309	
		C3 H8 N O2 S2	643	
		C52 H65 O3	909	
		C38 H67 N8 O8	987	

Name	CAS	Formula	Similarity	Class
		C49 H75 N4 S	719	
		C14 H39 N16 S	570	
		C51 H73 N4 O S	389	
		C47 H69 N4 O S	410	
		C40 H71 N6 O8	963	
		C31 H69 N11 O2 S	639	
		C46 H82 Cl N O7	622	
		C44 H66 N	949	
		C10 H8 N2 O2	930	
		C43 H78 N4 O2	952	

Influent particles GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ adipates					
DINP	28553-12-0	C26 H42 O4	704	Phthalate	344
Dibutyl phthalate	84-74-2	C16 H22 O4	935	Phthalate	305
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	C16 H22 O4	870	Phthalate	214
DEHP	117-81-7	C24 H38 O4	889	Phthalate	197
Diethyl Phthalate	84-66-2	C12 H14 O4	871	Phthalate	51
Benzyl butyl phthalate	85-68-7	C19 H20 O4	703	Phthalate	8,8
OP					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	750	OP	53
Triphenyl phosphate	115-86-6	C18 H15 O4 P	794	OP	20
Other polymer components/additives					
Oleamide	301-02-0	C18 H35 N O	897	Lupricant, slip agent	1337
Oleyl nitrile	112-91-4	C18 H33 N	897	Plasticizer, OLN	1183
2,6-di-t-butyl-p-benzoquinone	719-22-2	C14 H20 O2	774	Antioxidant (BHT quinone)	251
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	872	Antioxidant degr. Prod.; Keto-ester	236
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	880	Antioxidant	184
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	811	Benzothiazole	149
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	759	Benzothiazole	146
9-Octadecynenitrile	56599-96-3	C18 H31 N	763	Nitrile, platicizer in rubber	126
Benzenethiol, 3-methyl-	108-40-7	C7 H8 S	791	Thiol, aromatic	123
Butylated Hydroxytoluene	128-37-0	C15 H24 O	834	Antioxidant	129
Benzothiazole	95-16-9	C7 H5 N S	717	Benzothiazole	93
2-Benzothiazolamine, N-ethyl-	28291-69-2	C9 H10 N2 S	709	Benzothiazole	50
Benzenethiol	108-98-5	C6 H6 S	701	Thiol, aromatic	22
Disulfide, bis(4-methylphenyl)	103-19-5	C14 H14 S2	774	Disulfide, cross linking agent	16
PPCP + flavour/fragrances					
N,N-Dimethyldodecanamide	3007-53-2	C14 H29 N O	874	Surfactant, solvent	177

Acetophenone	98-86-2	C8 H8 O	708	Ketone, aromatic	42
N,N-Dimethyldecanamide	14433-76-2	C12 H25 N O	700	Surfactant, solvent	21
Halogenated compounds/ Pesticides					
3,5-Dichlorobenzoic acid	51-36-5	C7 H4Cl2 O2	703	Halogenated compound	11
PAC					
Phenanthrene	85-01-8	C14 H10	713	PAH	55
Fluoranthene	206-44-0	C16 H10	714	PAH	25
Pyrene	129-00-0	C16 H10	706	PAH	4,4

Influent particles LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Benomyl	17804-35-2	C14 H18 N4 O3	958	Fungicide
Pirimicarb	23103-98-2	C11 H18 N4 O2	944	Insecticide
Phthalates				
dibutyl phthalate		C16 H22 O4	964	phthalate
benzyl butyl phthalate		C19 H20 O4	825	phthalate
Ethanol, 2-butoxy-, phosphate (3:1)		C18 H39 O7 P	977	OP
Tributyl phosphate or triisobutyl phosphate		C12 H27 O4 P	983	OP
Chemical reagents				
Benzylamine	100-46-9	C7 H9 N	864	chemical reagent
Pharmaceuticals and biomolecules				
Aminocaproic acid	60-32-2	C6 H13 N O2	987	Antifibrinolytic
Amylnitrite	110-46-3	C5 H11 N O2	876	CoronaryDilator
ANCITABINE	10212-25-6	C9 H11 N3 O4	670	synthetic
Butoctamide	32838-26-9	C12 H25 N O2	989	Hypnotic
Cassaidine	26296-41-3	C24 H41 N O4	955	Cardiotonic
Cyprodenate	15585-86-1	C13 H25 N O2	993	Stimulant
Dacarbazine	891-98-6	C6 H10 N6 O	926	Antineoplastic
Deprostil	33813-84-2	C21 H38 O4	928	Prostaglandin
Dipyridamol	58-32-2	C24 H40 N8 O4	988	CoronaryDilator
Emylcamate	78-28-4	C7 H15 N O2	805	Tranquilizer
Guanine	73-40-5	C5 H5 N5 O	849	DiagnosticAid
Lidocaine-M (dimethylaniline)	87-62-7	C8 H11 N	990	ChemicalLocalAnesthetic
Monapterin		C9 H11 N5 O4	724	
Nicotinamide	98-92-0	C6 H6 N2 O	830	Vitamin
Ricinolic acid	141-22-0	C18 H34 O3	986	Biomolecule
Not identified				
		C9 H2 F8 N O9 S	651	

Name	CAS	Formula	Similarity	Class
		C9 H22 F10 N11 O2	654	
		C13 H25 N2 O8	658	
		C9 H14 O S3	662	
		C5 H F2 O8 S	664	
		C12 H25 N O S	664	
		C8 H9 Cl F N2 O S	666	
		C7 H10 Br F2 O2	671	
		C8 H21 F6 N11	673	
		C5 H F2 O8 S	674	
		C16 H41 N6	675	
		C9 H21 F N O4	678	
		C9 H19 F5 N8 O4	680	
		C7 H19 F N7 O2	681	
		C14 H35 F4 N15 O	681	
		C9 H22 N3 O5	684	
		C11 H29 N4 O2	685	
		C9 H14 F9 N2 O8	688	
		C7 H19 F N4 O3	690	
		C33 H70 F N2	690	
		C18 H39 F N O	694	
		C15 H31 F O3	695	
		C10 H17 F6 N2 O8	696	
		C4 H N2 O5 S	696	
		C9 H4 F9 O14	702	
		C7 H11 F8 N6 O5	705	
		C7 H14 F9 N6 O2	707	
		C7 H19 F3 N5	708	
		C8 H F3 N O10 S	711	
		C8 H2 F N O7	711	
		C9 H6 F O15	711	
		C7 H19 F N7 O2	711	
		C15 H14 F23 N4 O3	712	
		C15 H43 F N15 S	713	
		C7 H19 F3 N5	714	

Name	CAS	Formula	Similarity	Class
		C7 H16 F4 N4 O7	716	
		C5 H11 F2 O4 S	716	
		C8 H21 N6 O7	717	
		C4 H F3 O5 S	719	
		C8 H25 F2 N8	720	
		C6 H15 F2 N6	723	
		C9 H12 Cl F3 N13 O	725	
		C18 H39 F N O	733	
		C4 H8 F10 N7 O	736	
		C13 H36 F3 N12 O2	736	
		C10 H30 F6 N13	736	
		C11 H12 F12 N O11 S2	737	
		C5 H13 F N2 O3	740	
		C H F4 N2 O2 S3	741	
		C12 H23 F N O2	742	
		C6 H12 F2 N5 O2	744	
		C14 H8 F O2	745	
		C10 H8 N4 O3	753	
		C16 H37 N18	757	
		C7 H10 F12 N6 O2	759	
		C4 H5 F5 N2 O5	759	
		C5 H9 F3 N3	760	
		C6 H14 F6 N8 O3	760	
		C13 H8 N2 O2	761	
		C10 H17 F2 N O3	762	
		C14 H3 F11 N O4	762	
		C6 H5 F8 O10	771	
		C5 H10 F3 N3 O	771	
		C5 H12 F4 N3 O6	776	
		C7 H8 F5 N2 O4	777	
		C4 H7 F8 N4 O3	780	
		C8 H20 F N3 O3	783	
		C6 H2 F7 O7	784	
		C7 H18 F3 N5	791	

Name	CAS	Formula	Similarity	Class
		C9 H21 F N O4	793	
		C7 H17 F3 N5	799	
		C9 H22 N3 O5	805	
		C12 H5 F2 N3	805	
		C7 H18 F3 N5	809	
		C4 H7 F8 N4 O3	811	
		C9 H7 F6	832	
		C12 H5 F12 N3 O	846	
		C4 H12 F3 N4 O4	867	
		C10 H8 F2 N2 O2	869	
		C15 H18 F6 N2 O2 S2	876	
		C10 H10 F3 N4 O12	877	
		C3 H5 F11 N7	884	
		C5 H13 N3 O7	897	
		C26 H44 F	958	
		C11 H18 N3 O	652	
		C34 H60 N11	659	
		C18 H48 F5 N19 O4	663	
		C19 H49 F6 N14 O5	664	
		C7 H10 O2	671	
		C17 H48 F7 N21 O2	675	
		C15 H28 Cl F12 N14 O4	682	
		C16 H44 F5 N19 O3	682	
		C15 H7 F7 N O13 S5	702	
		C28 H63 F2 N10 O3	703	
		C30 H36 F N6 S4	728	
		C17 H F2 N2 O18 S2	742	
		C11 H31 F3 N12 O5	742	
		C28 H59 N11 O3	747	
		C18 H O20 S2	748	
		C32 H28 N2 S3	749	
		C28 H63 F4 N15 O	764	
		C10 F18 O9 S2	782	
		C26 H52 N6 O4	808	

Name	CAS	Formula	Similarity	Class
		C20 H52 N19 O3	812	
		C39 H29 F N3 O9	827	
		C25 H34 N4	829	
		C23 F N O19 S	830	
		C4 F2 N3 O	831	
		C25 H52 F3 N5	831	
		C13 H35 F3 N12 O6	833	
		C20 H48 F N8 O3	834	
		C38 H70 F10 N7	836	
		C19 H F5 O23	841	
		C19 H35 F2 N O S2	843	
		C8 H22 F N6 O6	846	
		C20 H40 N6 O2	847	
		C22 H43 F3 O2	847	
		C36 H64 F4 N4 S2	852	
		C13 H25 F N9 O	853	
		C9 H12 N3 O4	861	
		C10 H22 O4	862	
		C9 H17 F3 O2	862	
		C26 H55 N11 O2	863	
		C9 H17 F3 O2	865	
		C7 H22 F3 N8 O4	865	
		C6 H14 O4	866	
		C9 H17 F3 O2	867	
		C15 H39 F3 N12 O7	868	
		C10 H19 F3 O2	871	
		C7 H15 N O3	874	
		C10 F9 O12	876	
		C28 H55 N8 O4	877	
		C8 H9 N	878	
		C16 H34 O3	881	
		C32 H69 N14 O3	882	
		C4 H F N O7 S	890	
		C20 F7 N2 O18	892	

Name	CAS	Formula	Similarity	Class
		C10 H18 Cl F N5 S2	897	
		C18 H48 N8 O14	899	
		C21 F5 O20	900	
		C24 H2 F5 N7 O17	900	
		C22 H48 N3 O4	905	
		C18 H4 F14 O17	906	
		C25 H2 F3 N5 O19	909	
		C24 H34 O6 S	913	
		C28 H3 F6 N6 O15	913	
		C22 H41 F3 O11	917	
		C31 H68 F N4 O3 S	920	
		C16 H28 N3 O9	926	
		C20 H37 F3 O10	927	
		C16 F14 O16	928	
		C16 H22 O4	933	
		C36 H70 F N5 S	934	
		C21 H48 F2 N6 O S	937	
		C28 H59 N11 O2	940	
		C36 H72 F N8 O S	942	
		C39 F15 N O2	943	
		C13 H29 F4 N10 O3	944	
		C10 H28 F N9 O7	948	
		C14 H24 N3 O8	950	
		C22 H48 F2 N3 O3 S	951	
		C9 H21 F4 N10 O	951	
		C17 H9 F12 N O10	954	
		C13 H4 F9 N O10	955	
		C22 H42 N7	956	
		C16 H29 F3 N3 O3	959	
		C6 H14 F2 N3 O2 S	960	
		C19 H41 N3 O5 S	960	
		C24 H41 F2 N7	961	
		C19 H44 F2 N6 S	962	
		C15 F16 N2 O14	962	

Name	CAS	Formula	Similarity	Class
		C19 H36 O2	962	
		C22 H54 F N11 O4	963	
		C32 H64 F N8 O3 S	965	
		C17 H42 F3 N8 O9	967	
		C14 H32 F3 N15 O3	968	
		C29 H61 N11 O	969	
		C20 H47 F N10	969	
		C12 H29 F6 N12 O	970	
		C25 H55 F2 N5 O S	971	
		C23 H52 F N18	971	
		C10 H28 F3 N12 O2	972	
		C29 H59 N8 O	972	
		C10 H16 N3 O6	972	
		C30 H66 F2 N6 O7 S	973	
		C12 H21 F3 O6	973	
		C25 H49 F3 O3	974	
		C37 H75 F N3 O11	974	
		C21 H48 F2 N6 S	974	
		C18 H33 F3 O	975	
		C8 H21 F N7 O3	976	
		C32 H67 F2 N15 S	976	
		C6 H12 N2	977	
		C16 H37 F N7	977	
		C10 H16 O5	977	
		C26 H45 F O3 S	977	
		C21 H45 N	977	
		C38 H69 F2 N2 O2	977	
		C30 H62 F3 N5 O	978	
		C20 H43 N O2	978	
		C17 H37 N O2	979	
		C31 H69 F2 N8 O S	979	
		C26 H53 N8 O2	980	
		C19 H48 F N11 O	980	
		C19 H36 O3	980	

Name	CAS	Formula	Similarity	Class
		C16 H34 O4	980	
		C37 H79 F2 N11 O3 S	981	
		C16 H35 N O2	981	
		C23 H52 F2 N6 O S	981	
		C31 H69 F2 N8 O4 S	981	
		C22 H47 N	982	
		C23 H48 F2 N3 O4 S	982	
		C27 H55 F5 N7 S	982	
		C21 H41 F3 O2	982	
		C24 H54 F N18	983	
		C22 H42 F O8	983	
		C18 H32 O2	983	
		C18 H38 F N O	983	
		C19 H41 N	983	
		C34 H71 F2 N15 O S	983	
		C29 H65 F2 N8 O3 S	983	
		C11 H28 F5 N17	984	
		C17 H35 F N2 O7	984	
		C14 H33 F N7	984	
		C12 F22 N8 O8	985	
		C8 H18 O5	985	
		C18 H44 F7 N19 O2	985	
		C29 H59 N8 O6	986	
		C16 H37 F N7 O	986	
		C21 H47 F8 N11 O4	986	
		C12 H19 F3 O3	986	
		C25 H51 N8 O9	987	
		C12 H19 F3 O3	987	
		C19 H30 F2 N3 O2	987	
		C33 H64 N7 O3 S	987	
		C18 H41 F N7 O2	987	
		C21 H44 O4	987	
		C20 H42 O11	988	
		C20 H43 F N13 O2	989	

Name	CAS	Formula	Similarity	Class
		C10 H15 F3 O3	989	
		C10 H19 F3 O	989	
		C19 H42 F N8	989	
		C23 H46 N6 O4	989	
		C6 H3 F2 N4 O	989	
		C15 H21 F2 N4 O	989	
		C22 H37 N4 O	989	
		C15 H36 F5 N17 O2	990	
		C33 H67 F5 N7 O3 S	990	
		C13 H9 F26 N10 O	990	
		C25 H49 N O4	990	
		C33 H72 F N18 O5	990	
		C24 H50 F N O	991	
		C20 H38 F N3 O7	991	
		C10 H20 O4	991	
		C21 H46 F N8	991	
		C23 H47 N8 O8	991	
		C23 H41 N	991	
		C13 H32 F5 N17 O	991	
		C22 H45 F8 N18	991	
		C14 H36 F7 N19	992	
		C18 H38 O5	992	
		C36 H75 N4 O9	992	
		C23 H46 F3 N2 O7	992	
		C30 H60 N6 O10	992	
		C6 H13 N3 O2	992	
		C16 H40 F7 N19 O	992	
		C22 H51 F N10 O	992	
		C23 H48 O5	993	
		C14 H33 F N7 O6	993	
		C16 H39 F N6 O4	993	
		C16 H39 F N6 O4	993	
		C16 H39 F N6 O4	994	
		C28 H56 N6 O5	994	

Name	CAS	Formula	Similarity	Class
		C14 H30 O8	994	
		C32 H64 N6 O16	994	
		C22 H47 N O2	994	
		C21 H44 O4	994	
		C18 H34 O2	994	
		C16 H34 O9	994	
		C30 H55 N5 O5	995	
		C17 H28 O9	995	
		C38 H76 N6 O13	995	
		C12 H25 N O	995	
		C28 H56 N6 O14	995	
		C36 H64 F2 N3 O3	995	
		C23 H48 N2 O	996	
		C34 H68 N6 O12	996	
		C37 H54 F2 N9	996	
		C21 H31 F3 O9	998	
		C22 H43 F3 O5	998	
		C20 H39 F3 O4	999	
		C18 H32 O	999	

Effluent GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ adipates					
Dibutyl phthalate	84-74-2	C16 H22 O4	904	Phthalate	59
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	C16 H22 O4	876	Phthalate	28
Diethyl Phthalate	84-66-2	C12 H14 O4	924	Phthalate	19
Hexanedioic acid, mono(2-ethylhexyl)ester	4337-65-9	C14 H26 O4	749	Adipate	15
DEHP	117-81-7	C24 H38 O4	926	Phthalate	14
Benzyl butyl phthalate	85-68-7	C19 H20 O4	825	Phthalate	6,5
OP					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	888	OP	171
Ethanol, 2-butoxy-, phosphate (3:1)	78-51-3	C18 H39 O7 P	864	OP	52
1-Propanol, 2,3-dichloro-, phosphate (3:1)	78-43-3	C9 H15Cl6 O4 P	853	OP	24
Tri(2-chloroethyl) phosphate	115-96-8	C6 H12Cl3 O4 P	859	OP	6,2
Tributyl phosphate	126-73-8	C12 H27 O4 P	915	OP	3,7
Triphenyl phosphate	115-86-6	C18 H15 O4 P	794	OP	2,4
Triisobutyl phosphate	126-73-8	C12 H27 O4 P	776	OP	2,1
Other polymer components/additives					
Oleyl nitrile	112-91-4	C18 H33 N	907	Plasticizer, OLN	55
Oleamide	301-02-0	C18 H35 N O	779	Lupricant, slip agent	41
2-(Methylthio)phenyl isothiocyanate	51333-75-6	C8 H7 N S2	867	Isocyano	39
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	881	Antioxidant degr. Prod.; Keto-ester	35
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	897	Plasticizer	30
2,4,7,9-Tetramethyl-5-decyn-4,7-diol	126-86-3	C14 H26 O2	871	Defoamer (BASF)	23
Bisphenol A	2948-46-1	C12 H18 O2	825	Plastics additive	21
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	833	Benzothiazole	20
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	892	Antioxidant	14
4,6-di-tert-Butyl-m-cresol	719-22-2	C14 H20 O2	772	Antioxidant	14
Benzenesulfonamide, 4-methyl-	70-55-3	C7 H9 N O2 S	849	Plasticizer	14
Disulfide, bis(4-methylphenyl)	103-19-5	C14 H14 S2	762	Disulfide, cross linking agent	14
Benzenesulfonamide, N-ethyl-2-methyl-	1077-56-1	C9 H13 N O2 S	915	Plasticizer	13
Ethanone, 2,2-dimethoxy-1,2-diphenyl-	24650-42-8	C16 H16 O3	897	Plastics additive, UV photoinitiator	10

Name	CAS	Formula	Similarity	Class	ng/sample
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	C15 H22 O2	737	Antioxidant	9,0
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	856	Benzothiazole	8,4
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl-	1025-15-6	C12 H15 N3 O3	736	Plastics additive, crosslinker	7,0
Benzenesulfonamide, N-ethyl-4-methyl-	80-39-7	C9 H13 N O2 S	823	Plasticizer	6,9
2,6-Dimethylphenyl isocyanate	28556-81-2	C9 H9 N O	797	Isocyano	5,6
Benzenesulfonanilide	1678-25-7	C12 H11 N O2 S	817	Plasticizer	5,3
Cyclohexane, isocyanato-	3173-53-3	C7 H11 N O	878	Isocyano	4,9
Benzothiazole	95-16-9	C7 H5 N S	859	Benzothiazole	3,0
Bayer 28,589	728-40-5	C14 H21 N O3	742	Antioxidan	2,7
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	C16 H30 O4	808	Ester, plasticizer	1,5
Benzenemethanesulfonamide	4563-33-1	C7 H9 N O2 S	748	Plasticizer?	0,4
PPCP + flavour/fragrances					
N,N,N',N'-Tetraacetylethylenediamine (TAED)	10543-57-4	C10 H16 N2 O4	909	Peroxide bleach activator	65
Benzhydrol	91-01-0	C13 H12 O	914	Perfume fixative...	50
Benzophenone	119-61-9	C13 H10 O	878	PPCP	30
N,N-Dimethyldodecanamide	3007-53-2	C14 H29 N O	891	Surfactant, solvent	16
N,N-Dimethyldecanamide	14433-76-2	C12 H25 N O	894	Surfactant, solvent	11
Crotamiton	483-63-6	C13 H17 N O	886	PPCP	8,8
Tonalid	21145-77-7	C18 H26 O	737	PPCP	7,3
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	C13 H22 O3	815	Perfume (hedione) "jasmin aroma"	5,1
Cedrol	77-53-2	C15 H26 O	813	Terpenoid	3,2
Acetophenone	98-86-2	C8 H8 O	806	PPCP	1,7
Halogenated compounds/ Pesticides					
Diethyltoluamide (DEET)	134-62-3	C12 H17 N O	881	Pesticide	19
Glycols					
2-Propanol, 1-[1-methyl-2-(2-propenyloxy)ethoxy]-		C9 H18 O3	809	Glycole	14
2-Propanol, 1-[2-(2-methoxy-1-methylethoxy)-1-methylethoxy]-		C10 H22 O4	784	Glycole	12
Miscellaneous					
Ethanone, 1-[4-(1-hydroxy-1-methylethyl)phenyl]-		C11 H14 O2	743	Keto-alkohol	18
7-Nonenamide		C9 H17 N O	789	Amide	15
4-(t-Butyl)benzaldehyde	939-97-9	C11 H14 O	741	Aldehyde (aromatic)	1,1

Name	CAS	Formula	Similarity	Class	ng/sample
N-Phenylsuccinimide	83-25-0	C10 H9 N O2	783	Amide	0,7
PAC					
2-Acetyl-6-methoxynaphthalene	3900-45-6	C13 H12 O2	741	PAH derivative	12
1,8-Naphthalic anhydride	81-84-5	C12 H6 O3	717	PAH derivative	2,2
2,6-Diisopropylnaphthalene		C16 H20	735	Alkyl-PAH	1,5
2,6-Diisopropylnaphthalene		C16 H20	750	Alkyl-PAH	0,9

Effluent LC-MS

Name	CAS	Formula	Similarity	Class
Biocides/disinfectants				
3-Hydroxycarbofuran	16655-82-6	C12 H15 N O4	830	acaricide, insecticide, nematicide metabolite
Thiofanox-sulfone	39184-59-3	C9 H18 N2 O4 S	819	acaricide/insecticide metabolite
Benzylhydroxybenzoate	94-18-8	C14 H12 O3	966	Disinfectant
Benzylisothiocyanate	622-78-6	C8 H7 N S	902	Disinfectant
Tridemorph	24602-86-6	C19 H39 N O	987	Fungicide
Climbazole	38083-17-9	C15 H17 Cl N2 O2	987	Fungicide
Dodemorph	1593-77-7	C18 H35 N O	957	Fungicide
Quinoxyfen	124495-18-7	C15 H8 Cl2 F N O	887	Fungicide
Sorbic acid	110-44-1	C6 H8 O2	870	Fungicide
Kresoxim-methyl	143390-89-0	C18 H19 N O4	869	Fungicide
Bitertanol	55179-31-2	C20 H23 N3 O2	849	Fungicide
8-Hydroxychinolin	148-24-3	C9 H7 N O	843	Fungicide
Dodemorph	1593-77-7	C18 H35 N O	833	Fungicide
Propiconazole	60207-90-1	C15 H17 Cl2 N3 O2	829	Fungicide
Benomyl	17804-35-2	C14 H18 N4 O3	806	Fungicide
Methabenzthiazuron	18691-97-9	C10 H11 N3 O S	1000	Herbicide
Diethofencarb	87130-20-9	C14 H21 N O4	982	Herbicide
Bentranil	1022-46-4	C14 H9 N O2	942	herbicide
Imazamethabenz	81405-85-8	C16 H20 N2 O3	906	Herbicide
Cycluron	2163-69-1	C11 H22 N2 O	806	Herbicide
Crotamiton	483-63-6	C13 H17 N O	994	Scabicide
Butacarb	2655-19-8	C16 H25 N O2	981	Insecticide
Citronellal hydrate	107-75-5	C10 H20 O2	972	Insecticide
Bufencarb	8065-36-9	C13 H19 N O2	937	Insecticide
Butacarb	2655-19-8	C16 H25 N O2	905	Insecticide
Affinin	25394-57-4	C14 H23 N O	896	Insecticide
Pirimicarb	23103-98-2	C11 H18 N4 O2	877	Insecticide
Methoprene	40596-69-8	C19 H34 O3	871	Insecticide
Tetram (TM)	78-53-5	C10 H24 N O3 P S	857	Insecticide

Butacarb	2655-19-8	C16 H25 N O2	852	Insecticide
Monocrotophos	6923-22-4	C7 H14 N O5 P	833	Insecticide
Fenthion-sulphoxide	3761-41-9	C10 H15 O4 P S2	937	insecticide metabolite
Hexazinone		C12 H20 N4 O2	710	Herbicide
PCPs				
tolyltriazole	29385-43-1	C7 H7 N3	992	corrosion inhibitor (often added to dishwasher detergents)
benzotriazole	95-14-7	C6 H5 N3	899	corrosion inhibitor (often added to dishwasher detergents)
OP				
Tributyl phosphate	126-73-8	C12 H27 O4 P	697	flame retardant
Tributylphosphate	126-73-8	C12 H27 O4 P	985	Plasticizer
Chemical reagents				
3,4-Methylenedioxybenzoic acid (Piperonylic acid)	94-53-1	C8 H6 O4	858	chemical intermediate
Benzylamine	100-46-9	C7 H9 N	873	chemical reagent
benzothiazole	95-16-9	C7 H5 N S	900	
Phthalates				
DEHP	117-81-7	C24 H38 O4	970	phthalate
Dibutylphthalate		C16 H22 O4	994	
Pharmaceuticals/biomolecules				
Nandrolone phenpropionate	62-90-8	C27 H34 O3	937	Anabolic; synonym = Nandrolone-phenylpropionate;
Benhepazone	363-13-3	C15 H12 N2 O	990	Analgesic
Benzydamine	642-72-8	C19 H23 N3 O	958	Analgesic
Sulprosal	58703-77-8	C10 H12 O6 S	885	Analgesic
Phenazone	60-80-0	C11 H12 N2 O	875	Analgesic
Citrodisalyl		C21 H16 O11	869	Analgesic
Alminoprofen	39718-89-3	C13 H17 N O2	868	Analgesic
Morazone	6536-18-1	C23 H27 N3 O2	851	Analgesic
Azaprocin	448-34-0	C18 H24 N2 O	836	Analgesic
Profadol	428-37-5	C14 H21 N O	823	Analgesic
1,4-Diphenyl-3,5-pyrazolidinedione	557366	C15 H12 N2 O2	811	Analgesic; synonym = Phenopyrazone
Losartan	114798-26-4	C22 H23 Cl N6 O	995	angiotensin antagonist
Candesartan	139481-59-7	C24 H20 N6 O3	975	angiotensin antagonist
Eprosartan	133040-01-4	C23 H24 N2 O4 S	995	angiotensin antagonist,

				antihypertensive
Telmisartan	144701-48-4	C33 H30 N4 O2	886	angiotensin II antagonist, antihypertonic
Oxifentorex	4075-88-1	C17 H22 N O	993	Anorexic
Loxanast	69915-62-4	C14 H26 O2	871	Antiallergic
Imidocarb	27885-92-3	C19 H20 N6 O	996	Antiamebic
Bicalutamide	90357-06-5	C18 H14 F4 N2 O4 S	843	antiandrogen
Flecainide	54143-55-4	C17 H20 F6 N2 O3	951	Antiarrhythmic
Amafolone	50588-47-1	C19 H31 N O2	854	Antiarrhythmic
Azithromycin	83905-01-5	C38 H72 N2 O12	995	Antibiotic
Pyocyanine	85-66-5	C13 H10 N2 O	987	Antibiotic
Etisomicin	70639-48-4	C22 H43 N5 O7	909	Antibiotic
Clarithromycin	81103-11-9	C38 H69 N O13	891	Antibiotic
Cetocycline	53228-00-5	C22 H21 N O7	878	Antibiotic
Cefrotil	52231-20-6	C20 H22 N4 O4 S	872	Antibiotic
Betamicin Gentamycine B	36889-15-3	C19 H38 N4 O10	867	Antibiotic
Cephalosporin C	61-24-5	C16 H21 N3 O8 S	864	Antibiotic
Cefotaxime	63527-52-6	C16 H17 N5 O7 S2	861	Antibiotic
Streptomycin	57-92-1	C21 H39 N7 O12	859	Antibiotic
Phenoxymethylpenicillin	87-08-1	C16 H18 N2 O5 S	840	Antibiotic
Trovafloxacin	147059-72-1	C20 H15 F3 N4 O3	805	Antibiotic
Butaxamine	2922-20-5	C15 H25 N O3	985	Anticholesteremic
Gamolenic acid	506-26-3	C18 H30 O2	864	Anticholesteremic
Eritadenine	23918-98-1	C9 H11 N5 O4	828	Anticholesteremic
Gemcadiol	35449-36-6	C14 H30 O2	812	Anticholesteremic
Valethamat	90-22-2	C19 H32 N O2	845	Anticholinergic
Warfarin	81-81-2	C19 H16 O4	877	Anticoagulant Rodenticide
Valproic acid	99-66-1	C8 H16 O2	995	Anticonvulsant
10,11-Dihydroxycarbazepine	35079-97-1	C15 H14 N2 O3	988	Anticonvulsant
Lamotrigine	84057-84-1	C9 H7 Cl2 N5	987	Anticonvulsant
Gabapentin	60142-96-3	C9 H17 N O2	949	Anticonvulsant
Nonapyrimine	5626-36-8	C15 H24 N4	905	Anticonvulsant
Valproic acid	99-66-1	C8 H16 O2	850	Anticonvulsant
Carbenzide	3240-20-8	C11 H16 N2 O2	1000	Antidepressant

Citalopram	59729-33-8	C20 H21 F N2 O	989	Antidepressant
Amitriptyline	50-48-6	C20 H23 N	985	Antidepressant
Venlafaxine	93413-69-5	C17 H27 N O2	985	Antidepressant
Modaline	2856-74-8	C10 H15 N3	983	Antidepressant
Amitriptyline	50-48-6	C20 H23 N	977	Antidepressant
Tandamine	42408-80-0	C18 H26 N2 S	935	Antidepressant
Dothiepin	113-53-1	C19 H21 N S	892	Antidepressant
Melitracene	5118-29-6	C21 H25 N	866	Antidepressant
Venlafaxine	93413-69-5	C17 H27 N O2	845	Antidepressant
Valdipromide	52061-73-1	C11 H23 N O	840	Antidepressant
Minaprine	25905-77-5	C17 H22 N4 O	827	Antidepressant
Modaline	2856-74-8	C10 H15 N3	826	Antidepressant
Amezepin	60575-32-8	C18 H20 N2	805	Antidepressant
Carpipramine	5942-95-0	C28 H38 N4 O	802	Antidepressant
Norcitalopram	62498-67-3	C19 H19 F N2 O	826	antidepressant metabolite
Anisylbutamide	24535-67-9	C12 H18 N2 O4 S	922	Antidiabetic
Glybuzole	1492-02-0	C12 H15 N3 O2 S2	772	Antidiabetic
Aminocaproic acid	60-32-2	C6 H13 N O2	834	Antifibrinolytic
Iproheptin	13946-02-6	C11 H25 N	992	Antihistamine
Cetirizine	83881-51-0	C21 H25 Cl N2 O3	973	Antihistamine
Benzophenone	119-61-9	C13 H10 O	963	Antihistamine
Lisuride	18016-80-3	C20 H26 N4 O	922	Antihistamine
Tolpropamine	5632-44-0	C18 H23 N	862	Antihistamine
Fexofenadine	83799-24-0	C32 H39 N O4	989	antihistaminic
Valsartan	137862-53-4	C24 H29 N5 O3	992	Antihypertensive
Eplerenone	107724-20-9	C24 H30 O6	991	antihypertensive
Enalaprilat	76420-72-9	C18 H24 N2 O5	931	Antihypertensive
Amiquinsin-	13425-92-8	C11 H12 N2 O2	859	Antihypertensive
Pentopril	8294-03-6	C18 H23 N O5	761	Antihypertensive
Cedrin	6040-62-6	C15 H18 O6	852	Antimalarial
Fluconazole	86386-73-4	C13 H12 F2 N6 O	840	Antimycotic
Amorolfine	78613-35-1	C21 H35 N O	832	Antimycotic
Aminopterin	54-62-6	C19 H20 N8 O5	980	Antineoplastic
Inproquone	436-40-8	C16 H22 N2 O4	920	Antineoplastic
Etoglucid	1954-28-5	C12 H22 O6	855	Antineoplastic

Mycophenolic acid	24280-93-1	C17 H20 O6	839	Antineoplastic
Febuprol	3102-00-9	C13 H20 O3	801	Antineoplastic
Vinglyeinate	865-24-7	C48 H63 N5 O9	801	Antineoplastic
Dodecyl 3,4,5-trihydroxybenzoate	1166-52-5	C19 H30 O5	989	Antioxidant
Memantine	19982-08-2	C12 H21 N	956	Antiparkisonian
Dioxamate	3567-40-6	C15 H29 N O4	859	Antiparkisonian
Metixene	4969-02-2	C20 H23 N S	781	Antiparkisonian
Palmidrol	544-31-0	C18 H37 N O2	974	Antiphlogistic
Meclofenamic acid	644-62-2	C14 H11 Cl2 N O2	974	Antiphlogistic
Ximoprofen-	56187-89-4	C15 H19 N O3	933	Antiphlogistic
Clofenamic acid	4295-55-0	C13 H9 Cl2 N O2	877	Antiphlogistic
Palmidrol	544-31-0	C18 H37 N O2	838	Antiphlogistic
Iodphenazone	129-81-7	C11 H11 I N2 O	817	Antiphlogistic
Diflumidone	22736-85-2	C14 H11 F2 N O3 S	807	Antiphlogistic
Oletimol	5879-67-4	C15 H15 N O	947	Antirheumatic
Phenetidinomethanesulfonic acid		C9 H13 N O4 S	934	Antirheumatic
Secoverine	57558-44-8	C22 H35 N O2	860	Antispamotic
Flavamine	15686-60-9	C21 H23 N O2	833	Antispamotic
Aprofene	607-40-6	C21 H27 N O2	819	Antispamotic
Ethyldibunate	5560-69-0	C20 H28 O3 S	845	Antitussive
Noscapine	128-62-1	C22 H23 N O7	940	Antitussive Stimulant
Valaciclovir	124832-26-4	C13 H20 N6 O4	869	Antiviral
1,2,3,4-Tetrahydroharmane-3-carboxylic acid	5470-37-1	C13 H14 N2 O2	837	benzodiazepine receptor antagonist
Alprenolol	13655-52-2	C15 H23 N O2	991	Beta-Blocker
Dexpropranolol	5051-22-9	C16 H21 N O2	979	Beta-Blocker
Alprenolol	13655-52-2	C15 H23 N O2	935	Beta-Blocker
Dilevalol	75659-07-3	C19 H24 N2 O3	810	Beta-Blocker
Bisoprolol	66722-44-9	C18 H31 N O4	809	Beta-Blocker
Cholestenone	601-57-0	C27 H44 O	991	Biomolecule
Irone	79-69-6	C14 H22 O	859	Biomolecule
Agaricic acid	666-99-9	C22 H40 O7	847	Biomolecule
Caryophyllene	87-44-5	C15 H24	838	Biomolecule
Norharman	244-63-3	C11 H8 N2	837	Biomolecule
Hexoprenaline	3215-70-1	C22 H32 N2 O6	947	Bronchodilator
Doxaprost	51953-95-8	C21 H36 O4	937	Bronchodilator

Dimabefylline		C16 H19 N5 O2	800	Bronchodilator
Nifedipine	21829-25-4	C17 H18 N2 O6	876	CaAntagonist
Trimexiline	58757-61-2	C17 H29 N	935	CapillaryProtectant
Cassaidine	26296-41-3	C24 H41 N O4	838	Cardiotonic
Benafentrine	35135-01-4	C23 H27 N3 O3	824	Cardiotonic
Xibornol	13741-18-9	C18 H26 O	970	Chemotherapeutic
Amidapsone	3569-77-5	C13 H13 N3 O3 S	823	Chemotherapeutic
Ezetimibe	163222-33-1	C24 H21 F2 N O3	828	cholesterol resorption inhibitor
Simvastatin	79902-63-9	C25 H38 O5	874	cholesterol synthesis inhibitor
1-Hydroxytacrine	104675-29-8	C13 H14 N2 O	940	cholinergic, tacrine metabolite
Fenetradil	54063-39-7	C22 H36 N2 O3	995	CoronaryDilator
Hydrocortisone	50-23-7	C21 H30 O5	890	Corticoid
Mazipredone	13085-08-0	C26 H38 N2 O4	886	Corticoid
Flumoxonide	60135-22-0	C26 H34 F2 O7	872	Corticoid
Tixocortol	61951-99-3	C21 H30 O4 S	864	Corticoid
Oxisopred	18118-80-4	C21 H28 O6	863	Corticoid
Hydrocortisone	50-23-7	C21 H30 O5	852	Corticoid
Fluocortolone acetate	1176-82-5	C24 H31 F O5	830	Corticoid
Trihexylamine	102-86-3	C18 H39 N	982	Degrad.Product ofPhaseTransf.Catal.
Fluorescein	153954	C20 H12 O5	912	diagnostic (pancreas)
Disotenin	65717-97-7	C18 H26 N2 O5	871	DiagnosticAid
Epitiostanol	2363-58-8	C19 H30 O S	852	DiagnosticAid
Apiol	523-80-8	C12 H14 O4	866	Diuretic
Canrenone	976-71-6	C22 H28 O3	838	Diuretic
Canrenone	976-71-6	C22 H28 O3	815	Diuretic
17 a-Estradiol	50-28-2	C18 H24 O2	991	Estrogen
Benzestrol	85-95-0	C20 H26 O2	905	Estrogen
Epiestriol	547-81-9	C18 H24 O3	854	Estrogen
Carboprost	35700-23-3	C21 H36 O5	821	Gynecologic
Enoxacin	74011-58-8	C15 H17 F N4 O3	866	Gyrase inhibitor
Lamtidine	73278-54-3	C18 H28 N6 O	825	H2-Blocker
2,5-Dimethoxyphenethylamine	3600-86-0	C10 H15 N O2	981	hallucinogen, illicit drug
1-Naphthylamine-4-sulfonic acid	84-86-6	C10 H9 N O3 S	884	Hemostatic
Atazanavir	198904-31-3	C38 H52 N6 O7	986	HIV protease inhibitor
Aldosterone	52-39-1	C21 H28 O5	831	Hormone

5-Hydroxy-DL-tryptophan	56-69-9	C11 H12 N2 O3	862	Hypnotic
Thiobarbital	77-32-7	C8 H12 N2 O2 S	842	Hypnotic
Valdetamide	512-48-1	C9 H17 N O	830	Hypnotic;Sedative
3,4-Methylenedioxyethamphetamine (MDEA)	14089-52-2	C12 H17 N O2	802	illegal drug, hallucinogen;Psychedelic;DesignerDrug; synonym = 3,4-Methylenedioxyethamphetamine (MDE)
Mizoribine		C9 H13 N3 O6	949	Immuno suppressant
Physcion	521-61-9	C16 H12 O5	933	Laxative
4-(n-Butylamino)benzoic acid	4740-24-3	C11 H15 N O2	996	local anesthetic metabolite
Tixocortol 21-pivalate	55560-96-8	C26 H38 O5 S	842	local corticoid
Cocaine	50-36-2	C17 H21 N O4	991	LocalAnesthetic
Pyromecaine	30103-44-7	C18 H28 N2 O	967	LocalAnesthetic
Paridocaine	7162-37-0	C17 H26 N2 O2	862	LocalAnesthetic
Butethamine	2090-89-3	C13 H20 N2 O2	833	LocalAnesthetic
Prilocaine	721-50-6	C13 H20 N2 O	825	LocalAnesthetic
Amylocaine	644-26-8	C14 H21 N O2	822	LocalAnesthetic
Ecgonine	481-37-8	C9 H15 N O3	806	LocalAnesthetic
Butoxycaine	2350-32-5	C17 H27 N O3	911	LocalAnesthetic; synonym = Stadacaine
Promoxolane	470-43-9	C10 H20 O3	995	Muscle relaxant
Isomylamine	28815-27-2	C18 H35 N O2	871	Muscle relaxant
Idrocilamide	6961-46-2	C11 H13 N O2	850	Muscle relaxant
Quetiapine	111974-69-7	C21 H25 N3 O2 S	974	neuroleptic
Cinitapride	66564-14-5	C21 H30 N4 O4	908	Neuroleptic
Sertindole	106516-24-9	C24 H26 Cl F N4 O	879	neuroleptic
Pipamperone	1893-33-0	C21 H30 F N3 O2	825	Neuroleptic
Alpertine	27076-46-6	C25 H31 N3 O4	825	Neuroleptic
3-Methyl-2-oxopentanoic acid	39748-49-7	C6 H10 O3	817	nutrition therapy, renal insufficiency
Codeine	76-57-3	C18 H21 N O3	844	Opioid
7-Oxomeptazinol	59263-74-0	C15 H21 N O2	842	opioid analgesic metabolite
Octamylamine	502-59-0	C13 H29 N	994	Parasympatholytic
Arpenal	298-60-2	C21 H28 N2 O	988	Parasympatholytic
Butylscopolaminium		C21 H30 N O4	820	Parasympatholytic
Alverine	150-59-4	C20 H27 N	806	Parasympatholytic

Oxyphenonium	14214-84-7	C21 H34 N O3	829	parasympatholytic, spasmolytic
Ethephon	16672-87-0	C2 H6 Cl O3 P	871	plant growth regulator
Chlorsuperlutin	6799-23-1	C24 H29 Cl O4	969	Progestin
Anagestone	2740-52-5	C22 H34 O2	962	Progestin
Deprostil	33813-84-2	C21 H38 O4	938	Prostaglandin
Deprostil	33813-84-2	C21 H38 O4	899	Prostaglandin
Vinconate	70704-03-9	C18 H20 N2 O2	881	Psychotropic
Camphorsulfonic acid	5872-08-2	C10 H16 O4 S	927	Respiration stimulant
Dihydroxymethylphenylbutyne	2033-94-5	C11 H12 O2	990	Sedative
Didrovaltrate	18296-45-2	C22 H32 O8	841	Sedative
Valperinol	64860-67-9	C16 H27 N O4	804	Sedative
Apronalide	528-92-7	C9 H16 N2 O2	803	Sedative
Cyprodenate	15585-86-1	C13 H25 N O2	998	Stimulant
Leptacline	5005-72-1	C12 H23 N	998	Stimulant
Cyprodenate	15585-86-1	C13 H25 N O2	995	Stimulant
Pyritinol	1098-97-1	C16 H20 N2 O4 S2	937	Stimulant
Hexocyclonic acid	7491-42-1	C9 H16 O3	869	Stimulant
Bemegride	64-65-3	C8 H13 N O2	808	Stimulant
Octodrine	543-82-8	C8 H19 N	998	Sympathomimetic
N-Benzylamphetamine	57378-23-1	C16 H19 N	915	Sympathomimetic
3-Phenylpropylamine	2038-57-5	C9 H13 N	868	Sympathomimetic
N-Isopropylamphetamine	66470-73-3	C12 H19 N	835	Sympathomimetic
Adrenone	99-45-6	C9 H11 N O3	829	Sympathomimetic
Clopidogrel	113665-84-2	C16 H16 Cl N O2 S	901	Thromb.aggr.inhib.
Valnoetamide	4171-13-5	C8 H17 N O	846	Tranquilizer
Clobazam	22316-47-8	C16 H13 Cl N2 O2	842	Tranquilizer
Sulnidazole	51022-76-5	C9 H14 N4 O3 S	838	Trichomonacide
Probenecid	57-66-9	C13 H19 N O4 S	912	Uriosuric
Xylometazoline	526-36-3	C16 H24 N2	975	Vasoconstrictor
Fenoxazoline	4846-91-7	C13 H18 N2 O	874	Vasoconstrictor
Pentifylline	1028-33-7	C13 H20 N4 O2	950	Vasodilator
Hexadiline	3626-67-3	C19 H33 N	890	Vasodilator
Zolertine	4004-94-8	C13 H18 N6	809	Vasodilator
Efloxate	119-41-5	C19 H16 O5	807	Vasodilator
Aciclovir		C8 H11 N5 O3	924	Virucide

Dimepranol	53657-16-2	C5 H13 N O	867	Virucide
Ritonavir	155213-67-5	C37 H48 N6 O5 S2	979	virustatic
4'-Hydroxynordiazepam		C15 H11 Cl N2 O2	994	
5-Allyl-5-cylcopentenylbarbituric acid		C12 H14 N2 O3	986	
Diisopropyl adipate	6938-94-9	C12 H22 O4	966	
Azoxystrobin		C22 H17 N3 O5	924	
Estradiol diacetate	3434-88-6	C22 H28 O4	871	
Ethinylcyclohexanol	78-27-3	C8 H12 O	809	
Ethyl 10-iodostearate	18672-39-4	C20 H39 I O2	804	
Ethyl 2-acetyl-3-oxotetradecanoate		C18 H32 O4	905	
Irbesartan		C25 H28 N6 O	913	
N-Butyl-3-(1-naphthoyl)indole	208987-48-8	C23 H21 N O	850	
Phenanthryl methyl hydantoin		C15 H14 N2 O2	840	
Spiroxasone	6673-97-8	C24 H34 O3 S	923	
Sulfacinnamine		C15 H14 N2 O2 S	822	
Not identified				
		C10 H12 N2 O2 S	1000	
		C10 H24 N4 S	1000	
		C10 H9 N O S2	1000	
		C12 H10 O15	1000	
		C12 H15 N5	1000	
		C12 H2 N2 S2	1000	
		C12 H29 N3 O12	1000	
		C12 H5 N5 O9 S2	1000	
		C13 H12 O4	1000	
		C13 H13 N3 O5	1000	
		C13 H8 O14 S2	1000	
		C14 H15 N S	1000	
		C14 H27 N	1000	
		C15 H10 N2 O13 S	1000	
		C15 H21 N3 O16 S2	1000	
		C15 H34 Cl2 N4 O5 S	1000	
		C16 H12 N2 O19	1000	
		C16 H12 N2 O19	1000	

C16 H27 N3 O S	1000
C16 H31 N O20 S	1000
C16 H32 N2 S	1000
C16 H38 N4 O14 S	1000
C16 H9 N5 O12	1000
C18 H11 N3 O4	1000
C18 H14 O10 S	1000
C18 H28 N4 O17 S2	1000
C19 H29 N3 O20	1000
C20 H2 N2 O24	1000
C24 H51 N3 O13 S	1000
C25 H4 N4 O7	1000
C30 H57 N	1000
C4 H N3 O S3	1000
C5 H14 Cl N5 O3	1000
C6 H10 N4 O6	1000
C7 H20 N4 O7	1000
C8 H11 Cl N2 O4	1000
C8 H13 N O7	1000
C9 H17 N O10	1000
C9 H7 N3 O4	1000
C12 H4 N2 O2 S	919
C25 H20 N2 O4	997
C6 H11 N5 O5	991
C28 H58 O5	988
C16 H3 N3 O18 S	987
C6 H2 N4 O6 S	979
C18 H5 N O10 S2	976
C17 H34 O11	971
C24 H42 N4 O2	971
C16 H25 N3 O10	965
C19 H28 N2 O9	965
C18 H11 N O3	961
C21 H32 Cl N O9	959
C9 H12 N2 O3 S	956

C19 H17 N5 O15 S	953
C6 H11 N5 O5	952
C10 H12 N2 O2 S	951
C16 H2 O2	945
C25 H7 Cl N4 O2 S	945
C17 H36 Cl N	940
C9 H17 N3 O7	931
C12 H25 N5 S	914
C9 H15 N3 O2 S	906
C16 H33 N5 O3	903
C15 H35 N3 O13	902
C21 H37 N O14	897
C24 H22 N2 O4	894
C18 H28 O	892
C4 H7 N3 O5 S2	889
C17 H10 N4 O6 S	882
C14 H21 N5 O8	871
C11 H15 Br N2 O14	870
C11 H22 N2 O5	869
C16 H6 O19	854
C11 H22 Br2 Cl N3 O2	853
C8 H2 N2 O8 S	853
C14 H4 O3	852
C18 H42 N6 O15 S2	851
C11 H3 N3 O3	842
C30 H52 Cl N O	838
C17 H5 N5	837
C7 H16 N8 O	835
C21 H40 N4 O5	834
C10 H16 O6	824
C6 H11 N5 O5	820
C7 H10 N4 O3 S	810
C9 H11 N3 O2 S	810
C5 H9 N3 O6 S	806

C12 H4 Cl3 N3 O5	800
C14 H18 Br Cl N2 S	800
C14 H27 Br2 N	800
C18 H N3 O17	800
C18 H40 N4 O5	800
C19 H45 N5 S	800
C25 H32 Br N3 O2 S4	800
C30 H66 Cl N5 O2 S2	800
C34 H48 Cl N O3 S3	800
C7 H3 Cl2 N O8 S	800
C7 H7 N5 O4	800
C8 H16 Cl2 N4 O4 S	800
C8 H6 Cl2 S	800
C16 H5 N5 O6	789
C18 H7 N3 O3 S2	788
C18 H28 O3 S2	785
C4 H12 N4 O3 S2	785
C9 H11 Br N2 O11 S	785
C16 H3 N3 O18 S	783
C24 H18 Cl3 N3 O	782
C6 H10 N2 O5 S	781
C19 H43 N3 O S	780
C8 H11 Cl2 N3 O S	777
C13 H3 N5 O10	774
C10 H5 N3 O7 S3	771
C14 H26 N2 O2 S3	770
C27 H54 O	770
C6 H N O4 S2	769
C20 H13 N5 O15	768
C26 H3 N5 O5	768
C11 H9 N5 O	766
C3 H8 Cl N3 O2 S	765
C11 H2 N2 O14 S	764

C21 H25 N O8	761
C15 H32 Br N	759
C19 H41 N3 O10 S2	756
C26 H19 N3	755
C25 H54 N2 O5	754
C26 H40 O3 S	749
C10 H9 N O5	747
C14 H30 Cl N O3	747
C12 H4 O12 S2	745
C16 H31 N3 O3	743
C7 H4 N2 O S2	743
C15 H27 Br O9 S2	741
C5 H9 N O6 S2	739
C11 H8 O14 S	738
C31 H58 N2 O	738
C33 H65 N3 O2	737
C8 H8 Br Cl4 N5 O7 S2	732
C11 Cl2 N2 O4 S2	725
C9 H5 N O8 S	725
C27 H36 Br N O S	720
C8 H12 S5	720
C20 H41 N O6 S	715
C9 H6 N4 O6	711
C15 H34 Br2 Cl N5 O3 S2	710
C3 H2 Cl N3 S2	708
C5 H2 Cl3 N S3	707
C6 H8 N4 O6	705
C10 H12 N2 O2 S	699
C14 H16 O16	697
C5 H9 Br4 N3 O S2	697
C20 H42 N4 O3	696
C13 Br Cl8 N3 O2 S	695
C10 H11 N5 O2	692

C20 H37 Br Cl2 N2 O9 S	691
C11 H20 N4	687
C13 H4 N2 S	687
C18 H26 N2 O15 S	685
C35 H49 Cl2 N3 O S	685
C6 H15 N O4 S	685
C24 H51 N O18 S	683
C9 H17 N3 O2 S	683
C6 H16 N4 O5	677
C12 H N O13	675
C16 H12 N2 O19	675
C32 H25 N3 O2	675
C4 H8 N2 O4 S3	675
C8 H19 N S3	675
C21 H36 N4 S4	673
C19 H10 Br Cl5 N4 O3 S	670
C6 H6 Br N5 S4	670
C14 H24 N2 S	665
C10 H3 N5 O S	664
C10 H2 N4 O5 S2	658
C13 H12 O5 S	658
C19 H43 Cl N4 O	658
C28 H9 N	655
C13 H30 N2 O2 S	654
C29 H57 N5 O	654
C9 Br Cl3 N2 O4	652
C8 H17 Cl2 N3	650
C13 H5 N3 O12 S	644
C9 H22 Br N3 O3 S2	643
C16 H38 N4 O14 S	640
C22 H10 O22	639
C8 H11 Br2 Cl N4 O7 S2	639

C28 H3 N O18 S	638
C32 H41 Cl5 N2	638
C15 H32 N2 O8	637
C14 H14 Cl2 N2 O5	633
C25 H18 O14	628
C4 H4 Br3 N O S	628
C18 H8	626
C18 H25 N5 O13 S	625
C8 H3 N3 O4	625
C4 H5 Cl N2 O2 S4	622
C10 H6 Br Cl N2 O13	620
C14 H2 O4 S2	620
C11 H23 Cl2 N5 O2 S4	619
C5 H2 Br2 Cl N O3	619
C17 H7 N3 O13 S3	617
C25 H18 N2 O3 S	616
C24 H41 N O7	613
C9 H19 N5 S	612
C9 H19 N5 O2	611
C8 H9 N5 O5	607
C15 H2 N2 O13	606
C4 H5 Br2 N3 O5 S	602
C21 H19 N3 O21	601
C11 H9 N5 O	600
C21 H6 N2 O16	600

Contaminated fjord GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Phthalates/ adipates					
DEHP	117-81-7	C24 H38 O4	933	Phthalate	423
Diethyl Phthalate	84-66-2	C12 H14 O4	942	Phthalate	110
Dibutyl phthalate	84-74-2	C16 H22 O4	943	Phthalate	85
Adipic acid, cyclopentylmethyl dodecyl ester	0-00-0	C24 H44 O4	755	Adipate	75
Dibutyl phthalate	84-69-5	C16 H22 O4	887	Phthalate	60
Adipic acid, butyl cyclohexyl ester	0-00-0	C16 H28 O4	829	Adipate	53
Adipic acid, cyclohexyl ethyl ester	0-00-0	C14 H24 O4	858	Adipate	51
DEHA	6938-94-9	C22 H42 O4	709	Adipate	22
Phthalic acid, ethyl pentyl ester		C15 H20 O4	860	Phthalate	21
Adipic acid, di(oct-4-yl ester)	0-00-0	C22 H42 O4	786	Adipate	19
Hexanedioic acid, mono(2-ethylhexyl)ester	4337-65-9	C14 H26 O4	713	DEHA monoester	18
Benzyl butyl phthalate	85-68-7	C19 H20 O4	713	Phthalate	12
Phthalic anhydride	85-44-9	C8 H4 O3	785	Phthalate	8,7
Adipic acid, cyclohexyl isobutyl ester	0-00-0	C16 H28 O4	713	Adipate	8,1
Diisooctyl adipate	1330-86-5	C22 H42 O4	729	Adipate	7,2
OP					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18Cl3 O4 P	738	OP	12
Tributyl phosphate	126-73-8	C12 H27 O4 P	764	OP	7,2
Triisobutyl phosphate		C12 H27 O4 P	826	OP	4,6
Triethyl phosphate	78-40-0	C6 H15 O4 P	742	OP	0,7
Other polymer components/additives					
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	C14 H20 O2	753	Antioxidant	389
Oleyl nitrile	112-91-4	C18 H33 N	907	Plasticizer, OLN	293
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	886	Benzothiazole	160
2-Mercaptobenzothiazole	149-30-4	C7 H5 N S2	868	Benzothiazole	128
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	864	Antioxidant degr. Prod.; Keto-ester	63
Benzothiazole	95-16-9	C7 H5 N S	922	Benzothiazole	49
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	885	Antioxidante	47

Name	CAS	Formula	Similarity	Class	ng/sample
1,4-Benzenediol, 2,6-bis(1,1-dimethylethyl)-	2444-28-2	C14 H22 O2	753	Antioxidant	44
Octanamide, N,N-dimethyl-	1118-92-9	C10 H21 N O	775	Surfactant, solvent	35
Benzothiazole, 2-chloro-	615-20-3	C7 H4Cl N S	878	Benzothiazole	16
Benzothiazole, 2-butyl-	54798-95-7	C11 H13 N S	702	Benzothiazole	15
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	C16 H30 O4	876	PVC plasticizer (Eastman TXIB)	14
Decanenitrile	1975-78-6	C10 H19 N	899	Nitirle	10
Phenol, 2,4-di-t-butyl-6-nitro-	20039-94-5	C14 H21 N O3	706	Antioxidante	4,2
Butylated Hydroxytoluene	128-37-0	C15 H24 O	712	Antioxidante	1,3
PPCP + flavour/fragrances					
2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	17092-92-1	C11 H16 O2	875	PPCP, fragrance	76
3-Oxo-á-ionone	98910-85-1	C13 H18 O2	801	PPCP, fragrance	35
Gamma-Nonanolactone	104-61-0	C11 H20 O2	799	Artificial flavour, "creamy/coconut"	18
Benzophenone	119-61-9	C13 H10 O	873	PPCP	15
Gamma-Hexalactone	695-06-7	C6 H10 O2	884	Artificial flavour, "waxy, creamy"	9,6
2(3H)-Furanone, 5-ethenyldihydro-5-methyl-	1073-11-6	C7 H10 O2	811	Artificial flavour, "fruity, minty"	7,5
Gamma-Octalactone	104-50-7	C8 H14 O2	799	Artificial flavour, "coconut"	7,0
Benzoic acid, 2-ethylhexyl ester		C15 H22 O2	797	PPCP, sunscreen	5,5
Gamma-Decalactone	706-14-9	C10 H18 O2	817	Artificial flavour, "peach/apricot flavour"	5,0
Gamma-Heptalactone	105-21-5	C7 H12 O2	838	Artificial flavour, "coconut"	4,8
2(3H)-Furanone, 5-ethyldihydro-5-methyl-	2865-82-9	C7 H12 O2	765	Flavour/fragrance?	4,4
Ambrox	100679-85-4	C16 H28 O	705	PPCP, fragrance	1,5
Halogenated compounds/ Pesticides					
5-Chloropentanoic acid, cyclohexyl ester		C11 H19Cl O2	862	Halogenated compound	249
Cyclohexanone, 2-chloro-	822-87-7	C6 H9Cl O	934	Halogenated compound	168
Decachlorobiphenyl		C12Cl10	808	PCB	107
2-Chlorocyclohexanol	1561-86-0	C6 H11Cl O	940	Alkohol	84
5-Bromopentanoic acid, cyclohexyl ester	1554-79-6	C11 H19Br O2	792	Halogenated compound	36
Benzoic acid, 2,4-dichloro-	50-84-0	C7 H4Cl2 O2	701	Halogenated compound	25
Benzene, hexachloro-	118-74-1	C6Cl6	914	PCBz	24
Naphthalene, 1,2,3,4-tetrachloro-		C10 H4Cl4	832	PCN	15
1,1'-Biphenyl, 2,2',3,3',4,4',5,6,6'-nonachloro-	52663-79-3	C12 HCl9	702	PCB	14
Phenol, 2-chloro-	95-57-8	C6 H6 O	673	PCPh	8,6

Name	CAS	Formula	Similarity	Class	ng/sample
Benzene, pentachloro-	608-93-5	C6 HCl5	844	PCBz	5,9
Benzene, 1,2,3,4-tetrachloro-		C6 H2Cl4	818	PCBz	2,7
Various ketones, esters, aldehydes					
Benzeneacetic acid, cyclohexyl ester	42288-75-5	C14 H18 O2	803	Ester, aromatic	127
Benzoic acid, cyclohexyl ester		C13 H16 O2	794	Ester, aromatic	57
Benzyl Benzoate	120-51-4	C14 H12 O2	729	Ester, aromatic	32
Ethanone, 1,1'-(1,3-phenylene)bis-		C10 H10 O2	887	Ketone (alpha), aromatic	30
Cyclohexanecarboxylic acid, cyclohexyl ester	15840-96-7	C13 H22 O2	828	Ester	11
Ethanone, 1-(3-methylphenyl)-	585-74-0	C9 H10 O	786	Ketone (alpha), aromatic	9,7
Benzeneacetic acid, à-oxo-, methyl ester		C9 H8 O3	824	Ester, aromatic	4,7
PAC					
8-Isopropyl-1,3-dimethylphenanthrene		C19 H20	847	Alkyl-PAH	541
Fluoranthene	206-44-0	C16 H10	916	PAH	451
Triphenylene		C18 H12	808	PAH	250
Benz[a]anthracene		C18 H12	860	PAH	240
9,10-Anthracenedione, 2-methyl-		C15 H10 O2	833	O-PAH	209
Acenaphthylene	208-96-8	C12 H8	663	PAH	202
Benz[a]anthracene		C18 H12	738	PAH	188
Fluorene	86-73-7	C13 H10	899	PAH	166
Phenanthrene	85-01-9	C14 H10	914	PAH	164
6H-Dibenzo[b,d]-pyran	229-95-8	C13 H10 O	855	O-PAH	138
Naphtho[2,1-b]furan, 1,2-dimethyl-		C14 H12 O	819	N-PAH	131
Benzo[ghi]fluoranthene	203-12-3	C18 H10	882	PAH	119
Pyrene		C16 H10	868	PAH	111
Chrysene		C18 H12	834	PAH	107
2-Isopropyl-10-methylphenanthrene	66552-97-4	C18 H18	837	Alkyl-PAH	106
Chrysene		C18 H12	708	PAH	101
1,1'-Biphenyl, 4-methyl-		C13 H12	922	Alkyl-PAH	98
Phenanthrene, 1,7-dimethyl-		C16 H14	872	Alkyl-PAH	88
9H-Fluorene, 4-methyl-		C14 H12	758	Alkyl-PAH	87
Bibenzyl	103-29-7	C14 H14	783	PAH	79
Benzo[b]naphtho[1,2-d]furan	239-30-5	C16 H10 O	846	O-PAH	77
Cyclopenta(def)phenanthrenone	5737-13-3	C15 H8 O	886	O-PAH	73
Pyrene, 1-methyl-		C17 H12	883	Alkyl-PAH	68

Name	CAS	Formula	Similarity	Class	ng/sample
9,10-Anthracenedione	84-65-1	C14 H8 O2	920	O-PAH	66
11H-Benzo[a]fluoren-11-one		C17 H10 O	834	O-PAH	66
Benzo[h]cinnoline	230-31-9	C12 H8 N2	818	N-PAH	61
Anthracene, 1-methyl-		C15 H12	899	Alkyl-PAH	57
Chrysene, 2-methyl-		C19 H14	875	Alkyl-PAH	57
Dibenzofuran	132-64-9	C12 H8 O	874	PAH	56
Anthracene, 1-methyl-		C15 H12	905	Alkyl-PAH	55
Benz(A)anthracene-7,12-dione		C18 H10 O2	852	Alkyl-PAH	54
11H-Benzo[a]fluoren-11-one		C17 H10 O	867	O-PAH	51
9H-Fluorene, 2,3-dimethyl-		C15 H14	755	Alkyl-PAH	49
Naphtho[2,1-b]furan, 1,2-dimethyl-		C14 H12 O	700	N-PAH	48
9H-Cyclopenta[a]pyrene		C19 H12	795	PAH	48
6H-Benz[de]anthracen-6-one		C17 H10 O	814	O-PAH	46
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	824	Alkyl-PAH	42
Phenanthrene, 2,5-dimethyl-		C16 H14	887	Alkyl-PAH	42
Anthracene, 1-methyl-		C15 H12	899	Alkyl-PAH	41
Pyrene, 1-methyl-		C17 H12	799	Alkyl-PAH	40
Phenanthrene, 3,6-dimethyl-		C16 H14	823	Alkyl-PAH	38
Phenanthrene, 1,7-dimethyl-		C16 H14	836	Alkyl-PAH	37
Benz[c]acridine	225-51-4	C17 H11 N	792	N-PAH	35
1,1'-Biphenyl, 4-methyl-		C13 H12	803	Alkyl-PAH	35
Benzo[b]naphtho[2,1-d]thiophene	239-35-0	C16 H10 S	872	S-PAH	35
Phenanthrene, 2,3,5-trimethyl-		C16 H14	820	Alkyl-PAH	35
Anthracene, 9-ethenyl-		C16 H12	889	Alkyl-PAH	35
Benz(a)anthracene, 8,12-dimethyl-		C20 H16	772	Alkyl-PAH	34
3-Phenyl-benzofuran	29909-72-6	C14 H10 O	806	O-PAH	31
Dibenzofuran, 4-methyl-		C13 H10 O	806	Alkyl-PAH	30
4H-Cyclopenta[def]phenanthrene	203-64-5	C15 H8 O	840	PAH	29
2-Phenylnaphthalene	35465-71-5	C16 H12	938	PAH	29
Chrysene, 2-methyl-		C19 H14	830	Alkyl-PAH	28
11H-Benzo[b]fluorene		C17 H12	753	PAH	27
2-Fluorenecarboxaldehyde		C14 H10 O	801	O-PAH	26
Biphenylene	259-79-0	C12 H8	897	PAH	26
Benzo[b]naphtho[1,2-d]furan	239-30-5	C16 H10 O	843	O-PAH	25
9H-Fluorene, 2-methyl-		C14 H12	840	Alkyl-PAH	23
Naphthalene, 1,4,5-trimethyl-		C20 H12	897	Alkyl-PAH	23

Name	CAS	Formula	Similarity	Class	ng/sample
Naphthalene, 1,7-dimethyl-		C12 H12	861	Alkyl-PAH	22
Phenanthrene, 2,3,5-trimethyl-		C16 H14	775	Alkyl-PAH	22
Benzo[b]naphtho[2,1-d]thiophene	239-35-0	C16 H10 S	700	S-PAH	21
Pyrene, 4-methyl-		C17 H12	719	Alkyl-PAH	18
Anthracene, 9-ethenyl-		C16 H12	810	Alkyl-PAH	17
6H-Benz[de]anthracen-6-one		C17 H10 O	911	O-PAH	17
Naphthalene, 1-methyl-		C11 H10	886	Alkyl-PAH	16
2-Fluorenecarboxaldehyde		C14 H10 O	824	O-PAH	15
Naphthalene, 2-methyl-		C11 H10	906	Alkyl-PAH	14
1,1'-Biphenyl, 3,4'-dimethyl-		C14 H14	800	Alkyl-PAH	13
Naphthalene, 1,7-dimethyl-		C12 H12	806	Alkyl-PAH	13
Naphthalene, 1,4,5-trimethyl-		C20 H12	839	Alkyl-PAH	13
11H-Benzo[b]fluorene		C17 H12	788	PAH	12
Naphthalene, 1,7-dimethyl-		C12 H12	906	Alkyl-PAH	12
Naphtho[2,1-b]furan, 1,2-dimethyl-		C14 H12 O	867	N-PAH	12
9H-Fluoren-9-one, 1-hydroxy-		C13 H8 O2	795	O-PAH	12
Naphtho[2,3-b]thiophene		C12 H8 S	849	S-PAH	10
2,6-Diisopropylnaphthalene		C16 H20	799	Alkyl-PAH	8,6
Benzo[b]naphtho[2,3-d]furan		C16 H10 O	794	O-PAH	8,6
Anthracene, 9-phenyl-		C20 H14	787	PAH	8,5
Pyrene		C16 H10	727	PAH	8,2
Dibenzothiophene sulfone	1016-05-3	C12 H8 O2 S	793	S/O-PAH	8,0
9H-Fluorene, 1-methyl-		C14 H12	790	Alkyl-PAH	7,8
Biphenyl	92-52-4	C12 H10	902	PAH	6,5
Naphtho[2,1-b]furan, 1,2-dimethyl-		C14 H12 O	768	N-PAH	6,4
1,8-Naphthalic anhydride	81-84-5	C12 H6 O3	821	O-PAH	6,2
Indene	95-13-6	C9 H8	771	PAH	5,7
Dibenzothiophene, 4-methyl-		C13 H10 S	812	S-PAH	5,7
2,6-Diisopropylnaphthalene		C16 H20	800	Alkyl-PAH	4,9
Phenaleno[1,9-bc]thiophene		C14 H8 S	764	S-PAH	4,7
1H-Indene, 1-methylene-		C10 H8	925	Alkyl-PAH	4,4
Xanthone	90-47-1	C13 H8 O2	788	O-PAH	3,8
Naphthalene, 1,7-dimethyl-		C12 H12	760	Alkyl-PAH	3,1
Naphthalene, 1,4,5-trimethyl-		C20 H12	793	Alkyl-PAH	3,1
Phenanthridine	229-87-8	C13 H9 N	749	N-PAH	1,5
1(3H)-Isobenzofuranone	87-41-2	C8 H6 O2	836	O-PAH	1,3

Name	CAS	Formula	Similarity	Class	ng/sample
2,6-Diisopropylnaphthalene		C16 H20	823	Alkyl-PAH	0,9

Contaminated fjord LC-MS

Name	CAS	Formula	Similarity	Class
Imazamethabenz	81405-85-8	C16 H20 N2 O3	789	Herbicide
PCPs				
benzotriazole	95-14-7	C6 H5 N3	678	corrosion inhibitor (often added to dishwasher detergents)
OPs				
Tributylphosphate	126-73-8	C12 H27 O4 P	788	Plasticizer
Pharmaceuticals and biomolecules				
Actinobolin	24397-89-5	C13 H20 N2 O6	684	Antibiotic
Canrenoic acid	4138-96-9	C22 H30 O4	779	Diuretic
Cassaidine	26296-41-3	C24 H41 N O4	651	Cardiotonic
Emorfazone	38957-41-4	C11 H17 N3 O3	765	Analgesic
Ethyldibunate	5560-69-0	C20 H28 O3 S	772	Antitussive
Fencibutirol	1489-37-4	C16 H22 O3	709	
Fluorandrenolone	1524-88-5	C24 H33 F O6	887	Corticoid; synonym = Fludroxycortide
Hexoprenaline	3215-70-1	C22 H32 N2 O6	713	Bronchodilator
Hexoprenaline	3215-70-1	C22 H32 N2 O6	686	Bronchodilator
Nilvadipine	75530-68-6	C19 H19 N3 O6	857	CaAntagonist
Protheobromine	50-39-5	C10 H14 N4 O3	732	Cardiotonic
Pyrinoline	1740-22-3	C27 H20 N4 O	697	Antiarrhythmic
Phthalates				
Dibutyl phthalate	84-74-2	C16 H22 O4	904	Phthalate
Diethyl Phthalate	84-66-2	C12 H14 O4	937	Phthalate
Not identified				
		C19 H41 N O2	992	
		C21 H43 F O7 S	989	
		C49 H94 F3 N5 O3 P S	987	
		C16 H35 N O2	985	
		C34 H68 N2 O10	983	

Name	CAS	Formula	Similarity	Class
		C33 H7 Cl2 N O5 P S2	982	
		C20 H47 N4 O11	982	
		C21 H30 N3 O10	979	
		C13 H25 N O2	979	
		C16 H39 N4 O9	977	
		C34 H69 F4 N O P S2	976	
		C30 H61 N4 O P S	974	
		C18 H12 F26 N4 O7 P	974	
		C18 H38 O4	972	
		C36 H66 F4 N3 O S	970	
		C15 H32 F3 N5 O3	970	
		C18 H12 F26 N4 O7 P	970	
		C19 H43 N4 O	967	
		C31 H62 N O6	966	
		C51 H37 N5 O6	961	
		C36 H67 F3 N3 O P S	961	
		C10 H19 F3 O2	960	
		C11 H Cl2 F N O5	960	
		C43 H84 F4 O9 S	959	
		C18 H13 F24 N2 O13	959	
		C34 H69 Cl N O7	957	
		C18 H13 F24 N2 O13	957	
		C24 H47 O4	955	
		C55 H95 F3 N4 O4 P	952	
		C11 H Cl2 F N O5	951	
		C23 H42 F2 O2 S	950	
		C11 H Cl2 F N O5	945	
		C43 H61 F2 O P	944	
		C33 H72 F N4 O4 S	944	
		C38 H71 F3 N3 O2 P S	943	
		C31 H62 N2 O4 P S	942	
		C16 H22 O4	939	
		C37 H71 F N3 O8 S	937	
		C35 H66 F3 N4 O3 S	937	

Name	CAS	Formula	Similarity	Class
		C13 H31 N4 O	937	
		C26 H54 N O3	936	
		C41 H81 N O9 P S	935	
		C20 H42 O5	934	
		C39 H61 N O6	933	
		C35 H76 F N4 O5 S	928	
		C13 H4 Cl2 F N2 O5	926	
		C32 H62 F N4 O5 S	923	
		C42 H85 F N5 O5 P S2	923	
		C50 H51 F3 N2 O6	912	
		C15 H2 N2 O3	912	
		C55 H44 F4 O2 P	911	
		C39 H13 F7 N4 O5	910	
		C13 H24 F4 O S	907	
		C47 H88 F7 N3 O S	905	
		C H5 Cl N2 O2 S	902	
		C20 H36 O4	900	
		C16 H3 Cl2 N2 O4	900	
		C16 H22 O4	900	
		C51 H101 F6 N3 O2 P S2	897	
		C2 H5 Cl F O S	896	
		C25 H49 F N2 O	895	
		C11 H16 O3	893	
		C16 H18 F2 O2	887	
		C24 H28 F4 N O S	886	
		C10 H24 F2 N3 O S	886	
		C16 H21 N2 O8 S	880	
		C14 H17 F O7 S	879	
		C20 H23 N3 O6	879	
		C31 H67 N4 O2 P S2	879	
		C11 H23 N4 O	875	
		C20 H39 N O	875	
		C13 H18 F2 O	872	
		C38 H82 F3 N5 O3 P S	871	

Name	CAS	Formula	Similarity	Class
		C4 H2 Cl3 F N O4	869	
		C28 H46 N3 O S	869	
		C13 H17 F3 N2 O3	862	
		C6 H3 F N3 O	860	
		C16 H20 F2 O	860	
		C46 H96 F3 N5 O5 S2	859	
		C12 H16 F2 O	858	
		C3 H2 Cl3 F N O3	856	
		C15 H33 N4 O	856	
		C15 H33 N4 O	856	
		C24 H38 N3 O14	855	
		C14 H19 F3 N2 O	855	
		C49 H99 F4 N4 O4 S2	853	
		C16 H34 O3	850	
		C10 H19 F3 O	847	
		C5 H4 F O2 P	845	
		C13 H23 N O2	845	
		C40 H80 F3 N O4 S	844	
		C24 H50 F N O	844	
		C15 H30 F O	843	
		C19 H40 O4	842	
		C38 H80 F3 N5 O S2	840	
		C20 H24 N2 O3 P	839	
		C14 H20 O3	835	
		C10 H19 F3 O	834	
		C30 H61 F N3 O2 S2	832	
		C20 H39 N4 O	832	
		C24 H42 F6 N5 O2	830	
		C H2 F N O4	829	
		C22 H32 F4 O4 S2	829	
		C31 H53 N4 O2 S	827	
		C10 H8 Cl N O2 S2	827	
		C19 H45 N4 O4	826	
		C14 H27 N O3	825	

Name	CAS	Formula	Similarity	Class
		C10 H20 O4	824	
		C19 H40 O4	822	
		C29 H57 O P S2	818	
		C21 H27 F2 O	817	
		C23 H34 F O	815	
		C15 H24 O3	815	
		C23 H52 F N4 O2 S	814	
		C24 H45 O4	814	
		C25 H33 F N O4 S	814	
		C45 H65 N O S	814	
		C25 H56 F N4 O3 S	814	
		C16 H20 F2 O	812	
		C36 H31 Cl2 N3 O3	812	
		C29 H28 F O3	810	
		C34 H67 N4 O2 S	810	
		C15 H9 O P S2	809	
		C25 H53 F2 N O3 P	808	
		C14 H17 F3 O	808	
		C15 H2 N2 O3	806	
		C17 H3 F O14 P S2	804	
		C35 H30 Cl F N3 O P S	803	
		C32 H57 F3 O2 S2	802	
		C39 H66 N2 O5	802	
		C21 H45 N4 O3	802	
		C22 H24 F2 N2 O2 P	800	
		C31 H59 N O2 S	799	
		C40 H85 F2 N4 O3 S2	799	
		C24 H47 F3 O3	798	
		C39 H31 Cl2 F2 O	798	
		C22 H25 F2 O3 P	798	
		C20 H37 N O	797	
		C24 H43 F O S	796	
		C8 H2 N2 O8	795	
		C29 H49 N4 O S	794	

Name	CAS	Formula	Similarity	Class
		C32 H63 N4 O3 S	793	
		C13 H23 N O2	793	
		C39 H71 F2 N O3 S	791	
		C35 H75 Cl N5 O8	790	
		C12 H27 F2 N5 O P	789	
		C22 H25 F4 N O3	788	
		C35 H56 N4 O3 S	788	
		C26 H53 F2 O4 P	788	
		C11 H3 F17 O7 P	788	
		C21 H21 F7 N O3	785	
		C44 H89 F4 N5 O4 S	784	
		C11 H15 F2 N2 O	783	
		C20 H47 N4 O5	783	
		C21 H27 F2 O	782	
		C22 H46 F N O	781	
		C19 H43 N2 O4	780	
		C23 H42 N5 O4	779	
		C15 H2 N2 O3	779	
		C32 H60 F5 N O P	777	
		C50 H68 F6 N2 O9	773	
		C11 H14 N3 O4	773	
		C16 H13 F4 N4 O2	772	
		C20 H22 F7 N O3	771	
		C22 H45 F N2 O5	770	
		C14 H22 N2 O3	768	
		C33 H64 N O6	766	
		C11 H5 F9 O15 P	766	
		C15 H2 N2 O3	764	
		C13 H20 F N O4	764	
		C23 H51 F N5 O6	764	
		C17 H20 O	764	
		C27 H56 F3 N4 O2 P	762	
		C11 H13 F3 O	759	
		C44 H71 Br Cl2 N5 O7	756	

Name	CAS	Formula	Similarity	Class
		C52 H77 N2 O6 S	754	
		C27 H51 F O3 S2	753	
		C38 H69 F2 N O2 S	749	
		C43 H86 F5 N4 O5 S2	748	
		C32 H61 N O3 S	746	
		C24 H47 F5 N O2	745	
		C19 H20 O4	742	
		C23 H20 F3 N4 O2	739	
		C15 H2 N2 O3	736	
		C31 H61 N4 O2 S	734	
		C24 H35 N2 O P	733	
		C29 H60 N2 O4 S2	733	
		C26 H47 F3 O2 P	732	
		C35 H62 Cl2 N3 O17	726	
		C42 H83 F4 N2 O4 S	726	
		C14 H27 O S	723	
		C H3 Br2 Cl N O2	723	
		C38 H60 F2 N O4	722	
		C10 H9 N3 O2	721	
		C11 H16 O3	720	
		C21 H44 O5	716	
		C28 H44 F3 N5 O	712	
		C27 H45 F3 N O	711	
		C15 H16 F2 O	706	
		C32 H61 N O2 S	706	
		C29 H54 F2 N O	706	
		C26 H45 F2 N3 O4	704	
		C19 H19 O P	701	
		C42 H30 Cl2 F O	700	
		C48 H83 F2 N5 O S	697	
		C30 H34 N O	696	
		C27 H54 F4 N3 O5 P	696	
		C26 H49 F2 N O	694	
		C30 H52 F6 O	689	

Name	CAS	Formula	Similarity	Class
		C19 H30 N3 O3 S	688	
		C41 H67 Cl5 O8	687	
		C37 H65 Cl O4	681	
		C12 H16 F2 O	680	
		C17 H18 N O	680	
		C27 H55 F2 N O3	680	
		C43 H81 F7 N5 O4	678	
		C12 H30 N4 O3	674	
		C14 H14 N4 O2	673	
		C5 H N O3 S	672	
		C34 H52 F2 N O2	668	
		C30 H58 Cl N2 O P	668	
		C11 H5 O3	667	
		C54 H102 N3 O11	667	
		C15 H2 N2 O3	666	
		C35 H76 F N4 O6 S	664	
		C9 H19 N O6	664	
		C8 H19 N3 O5	661	
		C20 H F2 N O16 S	659	
		C43 H90 F2 N2 O5 P S2	657	
		C13 H5 Cl F2 N O	657	
		C20 H40 N5 O S	656	
		C38 H67 Cl N O4	655	
		C49 H88 F9 N O P	655	
		C42 H84 Cl N5 O4	654	
		C17 H2 O5	652	
		C8 H7 N4 O8	652	
		C8 H7 N4 O8	650	
		C33 H53 N O2	650	

Prawns GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
Other polymer components/additives					
Phenol, 2,6-bis(1,1-dimethylethyl)-	128-39-2	C14 H22 O	885	Antioxidant	68
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	784	Plasticizer	1,7
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	868	S-PAH	46
Halogenated compounds/ Pesticides					
Benzeneacetamide, N,N-dimethyl-	126-94-8	C10 H13 N O	816	Herbicide (diphenamid)	5,3
PAC					
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	857	Alkyl-PAH	128
Phenanthrene, 2,3,5-trimethyl-		C17 H16	838	Alkyl-PAH	46
Phenanthrene, 1,7-dimethyl-		C16 H14	875	Alkyl-PAH	40
Phenanthrene, 2,3-dimethyl-		C16 H14	876	Alkyl-PAH	34
9-Fluorenone, 2.4-dimethyl-		C15 H14	815	O-PAH	33
6-Cyanoquinoline		C10 H6 N2	771	N-PAH	32
Phenanthrene, 2,3,5-trimethyl-		C17 H16	841	Alkyl-PAH	31
Anthracene, 1-methyl-		C15 H12	877	Alkyl-PAH	28
9H-Fluorene, 1-methyl-		C14 H12	920	Alkyl-PAH	24
Phenanthrene, 2,3,5-trimethyl-		C17 H16	756	Alkyl-PAH	24
Phenanthrene, 3,6-dimethyl-		C16 H14	865	Alkyl-PAH	24
4-Phenanthrenol, 1,2,3,4-tetrahydro-4-methyl-		C15 H16 O	799	O-PAH	22
9H-Fluoren-9-one, 2,3-dimethyl-		C15 H14	801	O-PAH	21
Anthracene, 1-methyl-		C15 H12	920	Alkyl-PAH	21
Phenanthrene, 3,6-dimethyl-		C16 H14	879	Alkyl-PAH	20
Phenanthrene	85-01-8	C14 H10	961	PAH	18
9H-Fluorene, 2,3-dimethyl-		C16 H14	771	Alkyl-PAH	15
Naphthalene, 1-methyl-7-(1-methylethyl)-		C14 H16	829	Alkyl-PAH	15
1,2,3,3a,8,9,9a,9b-Octahydrocyclopenta[def]phenanthrene		C15 H18	757	PAH	15
Naphthalene, 2-methyl-1-propyl-		C14 H16	895	Alkyl-PAH	15
Phenanthrene, 1-methyl-		C15 H12	895	Alkyl-PAH	9,8

Name	CAS	Formula	Similarity	Class	ng/sample
1H-Indene, 5-hexyl-2,3-dihydro-		C15 H22	760	Alkyl-PAH	8,7
Anthracene, 1,2,3,4-tetrahydro-		C15 H16	880	PAH	8,3
Phenanthrene, 2,5-dimethyl-		C16 H14	753	Alkyl-PAH	7,5
Anthracene, 9,10-dihydro-2-methyl-		C15 H14	861	Alkyl-PAH	7,1
Pyrene	129-00-0	C16 H10	822	PAH	7,0
9H-Fluorene, 1-methyl-		C14 H12	899	Alkyl-PAH	6,3
Naphtho[2,1-b]furan, 1,2-dimethyl-		C14 H12 O	759	O-PAH	5,6
Naphthalene, 1,6-dimethyl-		C12 H12	770	Alkyl-PAH	5,5
9,10-Dimethylanthracene		C16 H14	869	Alkyl-PAH	5,2
Anthracene, 2-ethyl-		C16 H14	769	Alkyl-PAH	5,1
Naphthalene, 2,3-dimethyl-		C12 H12	826	Alkyl-PAH	4,9
2,2'-Dimethylbiphenyl		C14 H14	790	Alkyl-PAH	4,7
Fluoranthene	206-44-0	C16 H10	859	PAH	4,6
2-Phenylnaphthalene	35465-71-5	C16 H12	842	PAH	4,5
1-Naphthalenecarbonitrile	86-53-3	C11 H7 N	859	N-PAH	4,3
Fluorene	86-73-7	C13 H10	789	PAH	3,1
Benzo[h]cinnoline		C12 H8 N2	845	N-PAH	2,7
Anthracene, 9,10-dihydro-		C14 H12	785	PAH	2,3
Bibenzyl		C14 H14	800	PAH	2,0
Phenanthrene, 1,2,3,4-tetrahydro-		C14 H14	770	Alkyl-PAH	1,8
2-Hydroxyfluorene		C13 H10 O	766	O-PAH	1,6
Naphthalene, 1,7-dimethyl-		C12 H12	801	Alkyl-PAH	0,6
Benzo[c]cinnoline, 4-methyl-		C13 H10 N2	794	N-PAH	0,3
1H-Indene, 1-methylene-		C10 H8	772	Alkyl-PAH	0,2

Prawns LC-MS

Name	CAS	Formula	Similarity	Class
OPs				
2-Propanol, 1-chloro-, phosphate (3:1)		C9 H18 Cl3 O4 P	601	OP
Tributyl phosphate or triisobutyl phosphate		C12 H27 O4 P	859	OP
Triphenyl phosphate		C18 H15 O4 P	657	OP
Biocides				
Atrazine-desethyl	6190-65-4	C6 H10 Cl N5	629	herbicide
Isopropalin	33820-53-0	C15 H23 N3 O4	887	Herbicide
Dodemorph	1593-77-7	C18 H35 N O	989	Fungicide
Rubijervine	79-58-3	C27 H43 N O2	905	Fungicide
Additives				
Benzothiazole		C7 H5 N S	667	benzothiazole
N-tert-butylbenzothiazole-2-sulphenamide (TBS)		C11 H14 N2 S2	774	benzothiazole
Hexyl dodecanoate	34316-64-8	C18 H36 O2	997	fragrances
Oleamide		C18 H35 N O	988	Lupricant, slip agent
Oleyl nitrile		C18 H33 N	760	Plasticizer, OLN
UV-360		C41 H50 N6 O2	600	benzotriazole
PFCs				
PFOS		C8 H F17 O3 S	653	PFCs
Phthalates				
dibutyl phthalate		C16 H22 O4	808	phthalate
Pharmaceuticals and biomolecules				
Acetylprocaine	6062-23-3	C15 H22 N2 O3	978	
Aminocaproic acid	60-32-2	C6 H13 N O2	995	Antifibrinolytic
Benzylthiouracil	33086-27-0	C11 H10 N2 O S	664	Thyreostatic
Bifepramide	70976-76-0	C21 H28 N2 O	793	Parasympatholytic
Buprenorphine	52485-79-7	C29 H41 N O4	784	Opioid
Cannabidiol (CBD)	13956-29-1	C21 H30 O2	843	Psychedelic
Carebastine	90729-42-3	C32 H37 N O4	853	Antihistamine
Citrulline	372-75-8	C6 H13 N3 O3	905	LiverProtective
Cropropamide	633-47-6	C13 H24 N2 O2	985	Stimulant

Name	CAS	Formula	Similarity	Class
Dehydroabietic acid	1740-19-8	C20 H28 O2	984	Ingredient of Colophony
Delanterone	63014-96-0	C20 H28 O	980	Antiandrogen
Dimepranol	53657-16-2	C5 H13 N O	999	Virucide
Dimetholizine	7008-00-6	C15 H24 N2 O2	988	Antihistamine
Etoprindole		C15 H21 N3 O	654	Antiphlogistic
Famciclovir	104227-87-4	C14 H19 N5 O4	654	virustatic
Fexofenadine	83799-24-0	C32 H39 N O4	895	antihistaminic
Guaiactamine	15687-23-7	C13 H21 N O2	985	Antispamotic
Hexapropymate	358-52-1	C10 H15 N O2	730	Sedative
Histidine	71-00-1	C6 H9 N3 O2	773	Stomachic
Homoprenorphine	16549-56-7	C28 H37 N O4	656	Analgesic
Isomylamine	28815-27-2	C18 H35 N O2	987	Muscle relaxant
Isotretinoin	4759-48-2	C20 H28 O2	986	Dermatic
Lidocaine		C14 H22 N2 O	773	
Lidoflazine	3416-26-0	C30 H35 F2 N3 O	923	Vasodilator
Lomifylline	10226-54-7	C13 H18 N4 O3	660	Vasodilator
Mebutamate	64-55-1	C10 H20 N2 O4	825	Antihypertensive
Morin		C15 H10 O7	701	
Naphazoline	835-31-4	C14 H14 N2	982	Vasoconstrictor
Nifurdazil	1145-46-4	C10 H12 N4 O5	980	Chemotherapeutic
Palmidrol	544-31-0	C18 H37 N O2	981	Antiphlogistic
Palmitamide	629-54-9	C16 H33 N O	983	FattyAcid
Pexantel	10001-13-5	C12 H22 N2 O	913	Anthelmintic
Pirmenol	68252-19-7	C22 H30 N2 O	801	Antiarrhythmic
Progesterone		C21 H30 O2	888	
Promegestone	34184-77-5	C22 H30 O2	986	Progestin
Propacetamol	66532-85-2	C14 H20 N2 O3	990	Analgesic
Rociverine	53716-44-2	C20 H37 N O3	763	Antispamotic
Rubixanthin	3763-55-1	C40 H56 O	875	Biomolecule
Stevaladil	1692-96-0	C27 H45 N O4	840	Cardiotonic
Tilorone	27591-97-5	C25 H34 N2 O3	713	Virucide
Tripelenamine	91-81-6	C16 H21 N3	990	Antihistamine
Vigabatrin	60643-86-9	C6 H11 N O2	866	Anticonvulsant

Name	CAS	Formula	Similarity	Class
Not identified				
		C31 H11 N11 O24	607	
		C11 H22 N2 O3	611	
		C35 H15 N5 O26	616	
		C5 H9 N O2	620	
		C28 H27 N O30 S2	620	
		C5 H13 N3 O	634	
		C8 H11 N3 O	636	
		C46 H76 O4 S	638	
		C50 H68 N4	642	
		C31 H69 N15 O8	648	
		C9 H2 N2 O3 S2	650	
		C9 H2 N2 O3 S2	652	
		C9 H25 N5 O S	652	
		C9 H2 N2 O3 S2	653	
		C7 H14 O9 S	654	
		C9 H2 N2 O3 S2	654	
		C10 H6 N4 O5	658	
		C33 H64 N18 O	658	
		C10 H13 N O6 S	659	
		C9 H2 N2 O3 S2	659	
		C5 H2 N2 O8 S	659	
		C10 H18 N8 O2	660	
		C9 H25 N5 O S	664	
		C32 H65 N19 O4	668	
		C18 H36 O	673	
		C9 H14 N6 O4	673	
		C41 H75 N5 O8	676	
		C15 H36 N4 O	677	
		C7 H17 N3 S	680	
		C38 H80 Cl N9 O4 S	683	
		C28 H23 N7 O23 S3	683	
		C15 H2 O5	685	
		C39 H73 N9 O7	686	

Name	CAS	Formula	Similarity	Class
		C6 H10 O9 S	686	
		C7 H19 N7 O2	687	
		C46 H87 N3 O2 S3	696	
		C38 H67 N15 O2	696	
		C12 H23 N3 S	698	
		C35 H67 N17 O2	700	
		C7 H2 N4 O5 S	702	
		C17 H35 N3 O	703	
		C12 H2 O9	705	
		C26 H8 Cl2 N6 S3	705	
		C8 H11 N5 O8	707	
		C9 H14 N6 O4	708	
		C20 H45 N9 O	708	
		C10 H28 N6 O2	709	
		C12 H24 Cl N3	711	
		C31 H65 N17 O4	712	
		C10 H2 N4 O5	714	
		C10 H16 N2 O7	715	
		C30 H63 N19 O4	716	
		C10 H6 N4 O5	720	
		C42 H67 N15	720	
		C36 H72 N16 S	720	
		C31 H23 N O30 S	722	
		C16 H33 N17	724	
		C28 H49 N5 O5 S	724	
		C42 H81 Cl2 N9 S	726	
		C52 H71 N5 O	727	
		C9 H14 N6 O4	735	
		C33 H66 Cl N3 O2	735	
		C29 H20 Cl N11 O19 S3	737	
		C15 H32 O3	737	
		C13 H35 N7	739	
		C25 H50 N16 O	740	

Name	CAS	Formula	Similarity	Class
		C6 H13 N9 O2	740	
		C31 H58 Cl N9	741	
		C9 H14 N6 O4	743	
		C9 H20 N2 O2	744	
		C9 H14 N6 O4	744	
		C41 H85 Cl2 N5 O4 S	745	
		C34 H19 N O30	746	
		C9 H18 N2 O4	747	
		C16 H33 N17 O	748	
		C17 H34 N2	748	
		C46 H69 Cl N2 O5	749	
		C10 H16 N2 O3	750	
		C13 H10	750	
		C29 H45 N7 O	751	
		C10 H23 N O5	752	
		C17 H37 N17	756	
		C5 H11 N O2	757	
		C28 H56 Cl N O3	758	
		C37 H79 N5 O6 S2	760	
		C36 H62 Cl N3 O2	762	
		C13 H23 N O S	764	
		C47 H65 Cl N6	766	
		C3 H9 N7	766	
		C11 H N3 O6	767	
		C17 H35 N5 S	767	
		C34 H75 N9 O7 S	768	
		C42 H72 N4 S2	770	
		C9 H2 N2 O3 S2	771	
		C11 H12 N2 O2	773	
		C28 H49 N3 O5	773	
		C23 H35 N9 O3	774	
		C21 H41 N O2 S	775	
		C16 H37 N19 O3	775	
		C42 H42 O2	775	

Name	CAS	Formula	Similarity	Class
		C38 H77 Cl N2 O3	776	
		C44 H85 Cl2 N O6	777	
		C21 H38 N4 O	777	
		C28 H47 N3 O5	778	
		C42 H79 N5 O6 S	779	
		C18 H37 N19 O3	781	
		C26 H58 Cl N9	781	
		C42 H72 N4 S2	783	
		C28 H51 N3 O5	784	
		C20 H41 N13 O2	785	
		C32 H64 Cl N3 O2	789	
		C27 H43 N7 O2	789	
		C35 H60 Cl N O3	791	
		C32 H38 N6	793	
		C27 H44 N2 S	794	
		C29 H45 N7 O2	794	
		C26 H37 N7 O2	797	
		C26 H42 O4	797	
		C26 H39 N9 O	797	
		C30 H41 N9 O	799	
		C19 H32 N2	799	
		C17 H32 O2 S	799	
		C26 H51 N O9	800	
		C23 H39 N3 O5	801	
		C13 H19 N5	802	
		C27 H53 N3 O S	803	
		C9 H16 O9	804	
		C25 H37 N7 O	806	
		C15 H37 N13 O5	806	
		C25 H43 N3 O5	807	
		C37 H64 Cl N3 O2	809	
		C27 H60 Cl N9	809	
		C26 H56 Cl N9	811	
		C35 H69 N5 O8	813	

Name	CAS	Formula	Similarity	Class
		C11 H14 N2 O3	813	
		C19 H39 N O2 S	814	
		C35 H62 Cl N3 O2	815	
		C10 H25 N5 O S2	816	
		C29 H60 Cl N3 O2	816	
		C6 H10 O9 S	819	
		C15 H22 N2 O2	820	
		C23 H38 O2	820	
		C20 H28 O2	822	
		C12 H31 N15	825	
		C15 H32 S	826	
		C11 H20 N2 O5	827	
		C6 H10 O9 S	828	
		C17 H41 N11 O5	829	
		C6 H10 O9 S	829	
		C23 H50 N2 O8	830	
		C29 H41 N7 O	831	
		C6 H10 O9 S	836	
		C34 H20 Cl N O30	837	
		C5 H13 N3 O	838	
		C18 H34 O2	839	
		C24 H54 Cl N9	841	
		C6 H10 O9 S	842	
		C17 H34 O2 S	842	
		C10 H22 N2 O3	844	
		C25 H45 N O3 S	846	
		C21 H45 N5 S	846	
		C19 H37 N O3 S	849	
		C53 H108 N8 O3	849	
		C11 H20 N2 O3	851	
		C20 H46 N8 O7 S	854	
		C32 H43 N7 O2 S	854	
		C25 H53 N9 S	858	
		C17 H47 N11 S3	859	

Name	CAS	Formula	Similarity	Class
		C15 H43 N19 S	862	
		C24 H47 N O4 S	866	
		C40 H85 N3 O2 S4	866	
		C13 H20 O	866	
		C26 H49 N3 O S3	869	
		C20 H41 N9 O3 S	869	
		C25 H54 Cl N9	870	
		C6 H19 N5 O3 S	872	
		C22 H32 O2	873	
		C20 H44 N10 O S	877	
		C19 H43 N7 O7	879	
		C38 H82 Cl N11 O S2	882	
		C14 H38 N12 O3 S	884	
		C25 H45 N3 S2	884	
		C37 H74 Cl N17 O4	885	
		C24 H49 N3 O5 S	888	
		C23 H45 N9 O4 S	890	
		C25 H49 N O4	890	
		C31 H56 N10 O3	892	
		C15 H26 N14	892	
		C15 H26 N14	893	
		C24 H53 N11 O2	900	
		C32 H67 N17 O2 S	901	
		C21 H44 O5	902	
		C28 H54 O4	902	
		C3 H9 N7	902	
		C55 H105 N11 O S	903	
		C16 H38 N12 O8	904	
		C12 H15 N S	905	
		C20 H37 N O	908	
		C24 H55 N7 S2	911	
		C18 H45 N9 O3 S	912	
		C45 H47 N3 O	915	
		C11 H22 N2 O3	916	

Name	CAS	Formula	Similarity	Class
		C12 H20 N2 O4	918	
		C9 H12 Cl N3 O2 S4	920	
		C9 H12 Cl N3 O2 S4	921	
		C40 H77 N O10	923	
		C29 H57 N5 O5	923	
		C26 H43 N3 O6 S	923	
		C16 H44 N10 O3	924	
		C25 H39 N7 O	924	
		C18 H41 N9 O9	924	
		C25 H37 N3 O6	924	
		C22 H40 N14 S	926	
		C42 H71 N7 O3 S	927	
		C15 H39 N13 O5	927	
		C37 H75 N3 O12	933	
		C28 H57 N5 O4	934	
		C30 H57 N15 O	936	
		C21 H43 N13 S	938	
		C32 H55 N11 O S	938	
		C60 H111 N5 O3 S	938	
		C21 H35 N9 O3	939	
		C23 H45 N O2	939	
		C15 H34 N10 O3 S	940	
		C22 H43 N5 O	940	
		C14 H40 N10 O2	941	
		C25 H41 N O2	943	
		C24 H47 N5 O2	943	
		C41 H65 Cl N6	944	
		C20 H49 N9 O3 S	945	
		C24 H54 Cl N11 O2	946	
		C27 H56 Cl N9	946	
		C9 H18 N2 O3	948	
		C25 H39 N7 O	949	
		C17 H35 N13 S	949	
		C25 H45 N3 O5	949	

Name	CAS	Formula	Similarity	Class
		C12 H36 N10 O	951	
		C53 H95 N3 O4	951	
		C12 H24 N2 O3	952	
		C8 H16 N2 O3	952	
		C31 H61 N5 O6	952	
		C22 H49 N9 O9	953	
		C33 H71 N9 O10	954	
		C45 H91 N9 O2	954	
		C20 H41 N13 S	955	
		C18 H38 O4	957	
		C24 H35 N O3	959	
		C29 H56 Cl N9	960	
		C22 H33 N O	962	
		C18 H44 N16 S	962	
		C26 H42 N4 O3	963	
		C20 H47 N9 O4 S	963	
		C28 H48 N4	965	
		C14 H27 N O	965	
		C28 H44 N4 O3	965	
		C16 H33 N O2	965	
		C19 H40 O4	965	
		C27 H49 N3 O5	965	
		C26 H52 N6 O7	966	
		C54 H103 N11 O S	967	
		C22 H41 N13 S	967	
		C20 H39 N13 S	968	
		C19 H30 N4 O5	968	
		C22 H34 N4 O5	969	
		C24 H47 N13 S	969	
		C36 H73 N7 O8	969	
		C54 H93 N7	969	
		C21 H41 N13 S	970	
		C26 H45 N3 O5	970	
		C21 H45 N13 S	971	

Name	CAS	Formula	Similarity	Class
		C9 H16 N4 O6	971	
		C44 H85 N15	971	
		C31 H66 Cl N19	971	
		C26 H43 N13 S	972	
		C30 H49 N3 O6	972	
		C43 H67 Cl N4 O2 S	973	
		C43 H78 N26 S	973	
		C12 H25 N O10	973	
		C29 H45 N O4	974	
		C26 H41 N O3	975	
		C24 H39 N13 S	975	
		C18 H35 N O3	976	
		C25 H47 N O4	976	
		C15 H31 N O2	978	
		C22 H38 O2	978	
		C16 H35 N O2	979	
		C50 H97 N5 O6	979	
		C20 H39 N O2	979	
		C20 H39 N O2	979	
		C30 H40 N4 O6	981	
		C30 H60 Cl N5 O4	981	
		C31 H62 Cl N3 O2	982	
		C33 H44 O10	982	
		C26 H45 N3 O5	982	
		C27 H51 N O4	983	
		C17 H28 O9	983	
		C53 H99 N O5 S	984	
		C21 H43 N O2	984	
		C18 H33 N O3	985	
		C44 H70 N16 O11	986	
		C23 H45 N11 O3	987	
		C16 H34 O3	988	
		C22 H31 N7	990	
		C19 H38 N2 O4	992	

Name	CAS	Formula	Similarity	Class
		C28 H56 N6 O8	994	
		C19 H28 N6 O9	994	

Cod liver GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
OP					
Tributyl phosphate	126-73-8	C18 H15 O4 P	740	OP	7,9
Other polymer components/additives					
Phenol, 2,4,6-tris(1-methylethyl)-	2934-07-8	C15 H24 O	759	Antioxidant	161
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	C15 H22 O2	896	Antioxidant	15
Bayer 28,589	728-40-5	C14 H21 N O3	803	Antioxidant	3,2
Halogenated compounds/ Pesticides					
1,1'-Biphenyl, 2,2',3,3',4,6'-hexachloro-		C12 H4Cl6	692	PCB	79
2,2',3,5,6,6'-Hexachloro-1,1'-biphenyl		C12 H4Cl6	749	PCB	64
1,1'-Biphenyl, 2,2',3,4,4',5,6'-Heptachloro-		C12 H3Cl7	792	PCB	35
1,1'-Biphenyl, 2,2',3,4,4',5,6'-Heptachloro-		C12 H3Cl7	792	PCB	35
1,1'-Biphenyl, 2,2',3,3',4,6,6'-heptachloro-		C12 H3Cl7	760	PCB	33
1,1'-Biphenyl, 2,2',3,3',4,6,6'-heptachloro-		C12 H3Cl7	760	PCB	23
1,1'-Biphenyl, 2,2',3,3',4,6'-hexachloro-		C12 H4Cl6	821	PCB	22
Benzoic acid, 2,4-dichloro-	50-84-0	C7 H4Cl2 O2	747	Halogenated compound	19
4,4'-DDD	72-54-8	C14 H10Cl4	717	Pesticide	17
o,p-DDD		C14 H10Cl4	775	Pesticide	12
p,p'-DDE	72-55-9	C14 H8Cl4	901	Pesticide	9,1
1,1'-Biphenyl, 2,3',4,4',6-Pentachloro-		C12 H5Cl5	700	PCB	6,0
1,1'-Biphenyl, 2,2',3,3',4,5',6'-heptachloro-		C12 H3Cl7	714	PCB	1,2
1,1'-Biphenyl, 2,2',4,4',5-pentachloro-		C12 H5Cl5	723	PCB	1,0

Cod liver LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Methoprene	40596-69-8	C19 H34 O3	965	Insecticide
OPs				
Tributylphosphate	126-73-8	C12 H27 O4 P	839	Plasticizer
Triphenyl phosphate		C18 H15 O4 P	945	OP
Phthalates				
dibutyl phthalate		C16 H22 O4	983	phthalate
Additives				
Benzothiazole		C7 H5 N S	829	benzothiazole
Oleamide		C18 H35 N O	979	Lupricant, slip agent
Sweeteners				
Isosteviol	27975-19-5	C20 H30 O3	894	Sweetener
Pharmaceuticals and biomolecules				
4-Hydroxy-19-nortestosterone	4721-69-1	C18 H26 O3	843	Anabolic
Epirizole	18694-40-1	C11 H14 N4 O2	770	Analgesic
Ethenzamide	938-73-8	C9 H11 N O2	873	Analgesic
Renanolone	565-99-1	C20 H30 O4	780	Anesthetic
Embelin	550-24-3	C17 H26 O4	891	Anthelmintic
Dimantine	124-28-7	C20 H43 N	983	Anthelmintic
Embelin	550-24-3	C17 H26 O4	996	Anthelmintic
Hydnocarpic acid	459-67-6	C16 H28 O2	953	Antibiotic
Gamolenic acid	506-26-3	C18 H30 O2	984	Anticholesteremic
Trimoprostil	69900-72-7	C23 H38 O4	988	Anticulcerative
Pheniprazine	55-52-7	C9 H14 N2	767	Antidepressant
Cartazolate	34966-41-1	C15 H22 N4 O2	792	Antidepressant
Pheniprazine	55-52-7	C9 H14 N2	846	Antidepressant
Minaprine	25905-77-5	C17 H22 N4 O	849	Antidepressant
Salsoline	89-31-6	C11 H15 N O2	705	Antihypertensive
Penprostene	61557-12-8	C21 H32 O5	765	Antihypertensive
Caprylicacid octanoic acid	124-07-2	C8 H16 O2	813	Antimycotic

Anaxirone	77658-97-0	C11 H15 N3 O5	732	Antineoplastic
Mepitiostane	21362-69-6	C25 H40 O2 S	859	Antineoplastic
Etoglucid	1954-28-5	C12 H22 O6	859	Antineoplastic
Carmantadine	38081-67-3	C14 H21 N O2	804	Antiparkisonian
Castelamarin		C9 H14 O3	977	Biomolecule
Zindotrine	56383-05-2	C11 H15 N5	836	Bronchodilator
Diprophylline	479-18-5	C10 H14 N4 O4	953	Bronchodilator
Dienestrol diacetate	84-19-5	C22 H22 O4	823	Estrogen
Carboprost	35700-23-3	C21 H36 O5	821	Gynecologic
Cotarnine	82-54-2	C12 H15 N O4	670	Hemostatic
Butabarbital (Secubarbital)	125-40-6	C10 H16 N2 O3	747	Hypnotic
Amiflamine	77518-07-1	C12 H20 N2	960	MAO inhibitor
Promoxolane	470-43-9	C10 H20 O3	704	Muscle relaxant
Eperisone	64840-90-0	C17 H25 N O	944	Muscle relaxant
Nornicotine	494-97-3	C9 H12 N2	857	nicotine metabolite
Amixetrine	24622-72-8	C17 H27 N O	987	Parasympatholytic
Enisoprost	81026-63-3	C22 H36 O5	810	Prostaglandin
Gemeprost	64318-79-2	C23 H38 O5	882	Prostaglandin
Deprostil	33813-84-2	C21 H38 O4	929	Prostaglandin
Misoprostol	59122-46-2	C22 H38 O5	952	Prostaglandin
DMCC (ECC)	16499-30-2	C9 H16 N2	909	Psychedelic
PCM	2201-40-3	C16 H23 N O	833	Psychedelic;DesignerDrug
Menthyl salicylate	89-46-3	C17 H24 O3	999	Rubefacient; synonym = Menthylsalicylat
Oxanamide	126-93-2	C8 H15 N O2	745	Tranquilizer
Procymate	13931-64-1	C10 H19 N O2	831	Tranquilizer
Tolpiprazole	20326-13-0	C17 H24 N4	839	Tranquilizer
Valnoetamide	4171-13-5	C8 H17 N O	971	Tranquilizer
Dimepranol	53657-16-2	C5 H13 N O	994	Virucide
Mexrenoate	41020-68-2	C24 H34 O6	763	
Ethyl 2-acetyl-3-oxotetradecanoate		C18 H32 O4	853	
9,10-Dihydroxystearic acid	120-87-6	C18 H36 O4	856	
Benderizine	59752-23-7	C28 H34 N2 O2	693	Antiarrhythmic
Tocofibrate	50465-39-9	C39 H59 Cl O4	733	Anticholesteremic
Carbenoxolone	5697-56-3	C34 H50 O7	706	Anticulcerative

Amezepin	60575-32-8	C18 H20 N2	678	Antidepressant
Undecylenic acid	112-38-9	C11 H20 O2	719	Antimycotic
Salbutamol	18559-94-9	C13 H21 N O3	683	Bronchodilator
Mixidine	27737-38-8	C15 H22 N2 O2	722	CoronaryDilator
Cephaeline	483-17-0	C28 H38 N2 O4	710	Emetic
Promethestrol dibutyrate	6193-27-7	C28 H38 O4	678	Estrogen
Tetracaine	94-24-6	C15 H24 N2 O2	664	LocalAnesthetic
Razobazam	78466-98-5	C14 H14 N4 O2	672	Nootropic

Not identified

C36 H63 Cl N2	664
C24 H49 Cl N12 O2	670
C39 H67 Cl3 N2	684
C29 H44 N10 O2	685
C31 H69 Cl N10 S3	686
C36 H44 N4 O	686
C34 H62 Cl2 N8 O2	696
C29 H58 Cl2 O3	699
C20 H4 O7	716
C26 H54 Cl2 N2 O3	720
C30 H65 Cl N6 O3 S2	723
C37 H48 N2 O2	728
C5 H2 N2 O8 S	735
C24 H53 Cl N4 O5	737
C26 H50 N6 O5	737
C19 H45 Cl N14 O2	739
C18 H34 O2	740
C29 H65 Cl N10 O2 S2	740
C15 H2 N2 O3	749
C31 H44 N8 O	750
C5 H2 N2 O8 S	751
C5 H2 N2 O8 S	753
C5 H2 N2 O8 S	755
C25 H40 N4 O3	755
C23 H46 Cl2 N10 O	757
C11 H33 N13 O	759

C15 H34 N20 O	761
C24 H40 N10	773
C31 H51 Cl N8 O	773
C37 H71 Cl3 O S	774
C31 H57 Cl N8 O4	777
C7 H6 N4 O5 S	777
C22 H42 N16	778
C22 H40 O3	779
C28 H42 N4 O	780
C22 H40 O3	780
C12 H31 N5 S	783
C28 H53 Cl N4 S	790
C28 H44 N4 O3	794
C35 H66 S4	798
C29 H24 Cl N5 O26 S2	817
C7 H2 Cl N3 O4 S	818
C7 H6 N4 O5 S	818
C7 H6 N4 O5 S	821
C8 H12 O3 S	837
C19 H34 O2	847
C16 H32 O2	858
C5 H2 N2 O8 S	869
C5 H4 N4	869
C23 H36 N4	872
C5 H2 N2 O8 S	873
C18 H31 Cl O2	874
C21 H43 Cl N4 S	887
C15 H2 N2 O3	897
C24 H30 S2	903
C21 H37 Cl N4	910
C25 H48 N4 O3 S	914
C5 H Cl2 N5 O6	920
C18 H34 O2	938
C24 H47 Cl N4 O2 S	940
C27 H44 N4 O3	956

C19 H42 N10 O S	960
C23 H46 N4 O3 S	980
C18 H34 O2	981

Common eider GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
OP					
Tributyl phosphate	126-73-8	C12 H27 O4 P	735	OP	5,2
Triphenyl phosphate	115-86-6	C18 H15 O4 P	740	OP	0,8
Other polymer components/additives					
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	C17 H24 O3	888	Antioxidant degr. Prod.; Keto-ester	437
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	C14 H20 O2	756	Antioxidant	134
2(3H)-Benzothiazolone	934-34-9	C15 H22 O2	896	Benzothiazole	108
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	893	Antioxidant	72
1,4-Benzenediol, 2,6-bis(1,1-dimethylethyl)-	2444-28-2	C14 H22 O2	766	Antioxidant	19
Butylated Hydroxytoluene	128-37-0	C15 H24 O	775	Antioxidant	17
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	709	Plasticiser	12
Tributyl acetylcitrate	77-90-7	C20 H34 O8	789	Plasticiser, antifoaming agent	38
Halogenated compounds/ Pesticides					
2,3',4,4',5',6-Hexachloro-1,1'-biphenyl		C12 H4Cl6	705	PCB	69
Benzoic acid, 2,4-dichloro-	50-84-0	C7 H4Cl2 O2	801	Halogenated compound	53
Benzene, hexachloro-	118-74-1	C6Cl6	712	Pesticide	7,3
p,p'-DDE	72-55-9	C14 H8Cl4	706	Pesticide	6,6
o,p'-DDE		C14 H8Cl4	864	Pesticide	5,9
PAC					
Pyrene	129-00-0	C16 H10	798	PAH	23
Phenanthrene	85-01-8	C14 H10	910	PAH	19
Fluorene	86-73-7	C13 H10	771	PAH	17
Fluoranthene	129-00-0	C16 H10	758	PAH	6,3

Common eider LC-MS

Name	CAS	Formula	Similarity	Class
Biocides				
Hydroxysimazine	03.11.2599	C7 H13 N5 O	699	herbicide metabolite
Atrazine-desethyl	6190-65-4	C6 H10 Cl N5	701	herbicide
8-Hydroxychinolin	148-24-3	C9 H7 N O	982	Fungicide
UV adsorbers				
UV-234		C30 H29 N3 O	834	benzotriazole
Pharmaceuticals and biomolecules				
10-methyl-heptadecanoic acid		C18 H36 O2	833	http://lipidmaps.org/data/get_lm_lipids_dbgif.php?LM_ID
2,3-Diphospho-D-Glyceric Acid	138-81-8	C3 H8 O10 P2	732	Geigy vol.3 p.112
3,3'-Dihydroxydibutylether	821-33-0	C8 H18 O3	976	Choleretic
7-Desoxycholic acid	83-44-3	C24 H40 O4	744	Choleretic
9,10,13-trihydroxy-11-octadecenoic acid		C18 H34 O5	757	
Alfadolone	14107-37-0	C21 H32 O4	963	Anesthetic
Androstendiol dipropionate	2297-30-5	C25 H38 O4	985	Anabolic
Benserazide	322-35-0	C10 H15 N3 O5	766	Antiparkisonian
Benserazide	322-35-0	C10 H15 N3 O5	899	Antiparkisonian
Cannabidiol (CBD)	13956-29-1	C21 H30 O2	995	Psychedelic
Carebastine	90729-42-3	C32 H37 N O4	821	Antihistamine
Carmofur	61422-45-5	C11 H16 F N3 O3	777	Antineoplastic
Carpindolol	39731-05-0	C19 H28 N2 O4	778	Beta-Blocker
Ciclactate	15145-14-9	C12 H22 O3	803	Antispamotic
Citrulline	372-75-8	C6 H13 N3 O3	923	LiverProtective
Dimepranol	53657-16-2	C5 H13 N O	998	Virucide
Diphenylmethoxyisopropylnortropane		C23 H29 N O	690	Antihistamine
Drostanolone	58-19-5	C20 H32 O2	991	Anabolic
Fexofenadine	83799-24-0	C32 H39 N O4	864	antihistaminic
Furofenac	56983-13-2	C12 H14 O3	975	Antiphlogistic
Geroquinol	10457-66-6	C16 H22 O2	681	RadiationProtectant
Histidine	71-00-1	C6 H9 N3 O2	854	Stomachic
Mebhydroline	524-81-2	C19 H20 N2	737	Antihistamine; synonym = Mebhydrolin; additional Pragst

Metaraminol	54-49-9	C9 H13 N O2	771	Sympathomimetic
Metogest	52279-58-0	C20 H30 O2	946	Dermatic
Motrazepam	29442-58-8	C17 H15 N3 O4	788	Tranquilizer
Mycophenolic acid	24280-93-1	C17 H20 O6	990	Antineoplastic
Nabilone	51022-71-0	C24 H36 O3	960	Tranquilizer
Phenazopyridine	94-78-0	C11 H11 N5	931	UrinaryAntiseptic
Prazitone	2409-26-9	C16 H19 N3 O3	890	Antidepressant
Progesterone		C21 H30 O2	996	
Promestriene	39219-28-8	C22 H32 O2	814	Corticoid
Propacetamol	66532-85-2	C14 H20 N2 O3	945	Analgesic
Quinprenaline	13757-97-6	C14 H18 N2 O2	983	Bronchodilator
Riboflavin	83-88-5	C17 H20 N4 O6	978	vitamin B2
Somantadine	79594-24-4	C14 H25 N	774	Virucide

Not identified

C9 H24 N4 O4	658
C15 H30 N2 O4	670
C9 H5 N3 O7	677
C5 H2 N2 O8 S	703
C10 H10 N6 O4	706
C7 H6 N4 O5 S	706
C5 H2 N2 O8 S	706
C14 H34 N6	707
C3 H2 Cl2 N4	709
C5 H2 N2 O8 S	712
C11 H16 N6 O3	719
C9 H4 O S	722
C5 H2 N2 O8 S	725
C12 H2 O9	728
C11 H24 N2 O2 S2	732
C10 H10 N2 O9	740
C5 H2 N2 O8 S	746
C5 H2 N2 O8 S	751
C13 H31 N7	755
C15 H22 O6	759
C15 H32 N4 O	759

C13 H22 N4 O3	760
C17 H24 N2	766
C12 H21 N5 O	770
C10 H29 N7 O	771
C11 H2 O6 S	776
C16 H15 N5	777
C35 H69 Cl N4 O7	780
C15 H2 N2 O3	784
C9 H6 N4 O S3	788
C35 H69 Cl N4 O7	790
C28 H63 Cl N14	790
C9 H22 N4 O4	790
C10 H19 N5 S	795
C16 H15 N5	801
C7 H6 N4 O5 S	802
C8 H20 N6 O3	810
C37 H71 Cl N4 O7	814
C8 H20 N6 O3	818
C10 H29 N7 O	838
C7 H6 N4 O5 S	842
C5 H2 N2 O8 S	850
C7 H6 N4 O5 S	859
C5 H2 N2 O8 S	860
C15 H2 N2 O3	861
C7 H6 N4 O5 S	862
C5 H2 N2 O8 S	869
C8 H2 O6 S2	882
C47 H65 Cl N6	951
C47 H65 Cl N2	964
C38 H39 N5	652
C38 H74 Cl N13 O3	653
C5 H9 N O	658
C34 H72 N14 O S	661
C31 H69 N21 O6	683

C31 H23 N O30 S	685
C29 H62 N16 O6 S	686
C35 H73 N15 O8	689
C5 H5 N3 O3	689
C35 H69 N15 O5	692
C32 H69 N19 O3	692
C42 H85 N O8 S2	693
C20 H49 N9 O S2	694
C8 H8 O	700
C17 H37 N15 O2 S	701
C18 H39 N13 O5	702
C12 H26 N2 O2 S	706
C15 H36 N4 O	707
C35 H76 N6 O9	707
C9 H8 O3	708
C35 H59 N23	709
C34 H65 N19 O4	711
C39 H71 N15 S	717
C35 H72 N12 O2 S	724
C30 H61 N25 O2	731
C30 H59 N25 O2	736
C46 H71 N9 O2	739
C36 H75 N15 S2	740
C34 H72 N14 O S	745
C6 H15 N O2	746
C29 H65 N13 O15	750
C24 H39 N9 O S	751
C19 H28 N10 S2	751
C29 H64 N20 O2	754
C28 H61 N15 O14	758
C31 H35 N13	758
C20 H39 N13 O2 S	761
C39 H85 N7 O S4	763
C32 H39 N9 O	772
C5 H13 N O	773

C42 H53 N5 O3	775
C27 H39 N7 O2	776
C25 H43 N5 O5 S	776
C11 H21 N O2 S3	777
C36 H47 N13	777
C16 H43 N13 O2 S	779
C19 H44 N12 O3 S	785
C26 H29 N13	786
C21 H35 N13 O2	787
C10 H15 N3 O5	787
C27 H35 N13	788
C36 H76 N4 O10	789
C22 H40 N12 O3	789
C27 H39 N3 O3	789
C10 H24 N2 O3	790
C34 H43 N3 O3	796
C22 H45 N13 O2	796
C17 H35 N5 O3	797
C26 H49 N5 O5 S	797
C34 H41 N9 O	798
C16 H35 N19 O3	799
C42 H86 Cl N5 O3 S2	806
C58 H81 N S2	810
C28 H43 N5 S	812
C28 H47 N7 O2 S	812
C10 H13 N5 O	813
C15 H17 N O2 S	815
C39 H80 O9 S	822
C32 H56 N12 O S	829
C23 H47 N13 O2 S	830
C28 H54 Cl N O6 S	831
C16 H30 O2	833
C8 H6	834
C42 H5 N5 O16	834

C8 H11 N3 O	841
C21 H45 N13 O2 S	849
C21 H43 N13 O2 S	849
C30 H45 N O4 S	851
C48 H79 N O5 S	853
C25 H35 N17 O	854
C6 H13 N O3	857
C25 H42 N12 S	858
C19 H36 N18 O S	861
C40 H5 N3 O19	863
C6 H9 N O S	866
C26 H47 N7 O4	868
C29 H41 N11	871
C38 H71 Cl N2 S	872
C58 H81 N S2	873
C28 H59 N3 O S3	875
C33 H7 N9 O17	878
C21 H32 N4	882
C27 H43 N11	883
C31 H45 N O4 S	885
C50 H77 N7 O3 S	887
C38 H74 Cl N15 O2	888
C37 H11 N3 O19	890
C10 H22 O4	893
C50 H77 N7 O3 S	895
C24 H45 N7 O4	896
C22 H43 N3 O6 S	897
C28 H41 N7 O2	901
C17 H42 N12 O3 S	902
C25 H45 N9 O4 S	902
C23 H45 N O4	905
C13 H17 N O9 S	908
C24 H38 O4	908
C20 H41 N13 S	912

C25 H46 N2 O9	917
C16 H39 N19 O3	919
C32 H6 N6 O18	919
C27 H41 N3 O6	922
C25 H37 N3 O6	923
C19 H34 N4	923
C17 H40 N18 O S	924
C15 H37 N13 O5	925
C18 H45 N13 O5	927
C16 H43 N19 O3	928
C31 H39 N3 O6	934
C22 H35 N9 O4 S	938
C9 H12 Cl N3 O2 S4	938
C27 H43 N3 O6	940
C22 H12 Cl2 O10 S2	941
C9 H12 Cl N3 O2 S4	943
C22 H40 N8 O9	943
C21 H47 N9 O9	946
C21 H45 N11 O	949
C20 H39 N13 S	953
C17 H32 O2	955
C22 H41 N13 S	956
C35 H68 N2 O8	958
C36 H54 N12 O	959
C20 H42 O5	962
C21 H43 N13 S	962
C24 H41 N3 O6	965
C17 H28 O9	965
C24 H45 N13 S	966
C21 H43 N13 S	967
C36 H72 N10 O3 S	968
C20 H37 N O4	968

C23 H45 N13 S	968
C35 H66 N4 O4 S	969
C32 H40 N6 O7	970
C26 H43 N13 S	971
C46 H75 N3 O7	973
C19 H28 N6 O9	973
C19 H39 N13 S	973
C19 H28 N2 O12	976
C27 H43 N O4	977
C26 H45 N13 S	977
C11 H9 N O2	978
C25 H47 N O4	978
C22 H46 O6	980
C46 H94 N14 O6	980
C47 H83 N3 O7 S	981
C21 H43 N13 S	981
C18 H32 O	985
C12 H16 N4 O2 S	986
C12 H12 N2 O2	986
C12 H20 O4	986
C38 H82 N22 O9	987
C17 H32 N2 O5	989
C16 H35 N O2	989
C43 H86 N6 O17	993
C11 H11 N O3	993
C12 H10 N4 O2	994
C43 H74 N26 S	995

Common shag GC-MS

Name	CAS	Formula	Similarity	Class	ng/sample
OP					
Tri(2-chloroethyl) phosphate	115-96-8	C6 H12Cl3 O4 P	747	OP	23
Tributyl phosphate	126-73-8	C12 H27 O4 P	724	OP	12
Triisobutyl phosphate		C12 H27 O4 P	873	OP	9,8
Triphenyl phosphate	115-86-6	C18 H15 O4 P	772	OP	7,7
Other polymer components/additives					
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	891	Benzothiazole	763
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	882	Antioxidant	235
Benzenesulfonamide, N-butyl-	3622-84-2	C10 H15 N O2 S	841	Plasticizer	9,4
Halogenated compounds/ Pesticides					
1,1'-Biphenyl, 2,2',3,3',4,6'-hexachloro-		C12 H4Cl6	834	PCB	115
1,1'-Biphenyl, 2,3',4,5,5'-pentachloro-		C12 H5Cl5	726	PCB	89
1,1'-Biphenyl, 2,2',3,3',4,6'-hexachloro-		C12 H4Cl6	811	PCB	54
2,3',4,4',5'-Pentachloro-1,1'-biphenyl		C12 H5Cl5	702	PCB	44
1,1'-Biphenyl, 2,2',3,3',4,6,6'-heptachloro-		C12 H3Cl7	704	PCB	27
3,4'-Dichlorobiphenyl		C12 H8Cl2	737	PCB	14
1,1'-Biphenyl, 2,2',3,3',4,5,5'-heptachloro-		C12 H3Cl7	701	PCB	2,4
3,4'-Dichlorobiphenyl		C12 H8Cl2	709	PCB	1,1
1,1'-Biphenyl, 2,2',3',4,5-Pentachloro-		C12 H5Cl5	739	PCB	0,9
1,1'-Biphenyl, 2,3',5,5'-tetrachloro-		C12 H6Cl4	733	PCB	0,6
p,p'-DDE	72-55-9	C14 H8Cl4	889	Pesticide	36
Benzene, hexachloro-	118-74-1	C6Cl6	669	Pesticide	3,0
PAC					
Phenanthrene	85-01-8	C14 H10	917	PAH	43
Pyrene	129-00-0	C16 H10	787	PAH	35

Common shag LC-MS

Name	CAS	Formula	Similarity	Class
Pharmaceuticals and biomolecules				
(22S)-1alpha,25-dihydroxy-22-ethoxy-26,27-dimethyl-23,24-tetradehydro-20-epivitamin D3 / (22S)-1alph		C31 H48 O4	769	
10-methyl-heptadecanoic acid		C18 H36 O2	998	
11-cis-Retinaldehyde	564-87-4	C20 H28 O	994	
11-keto pentadecanoic acid		C15 H28 O3	803	
12-METHOXY-4,4-BISNOR-5alpha-8,11,13-PODOCARPATRIEN-3-OL		C16 H22 O2	717	semisynthetic
17-hydroxy-heptadecanoic acid		C17 H34 O3	669	
17-methyl-6Z-octadecenoic acid		C19 H36 O2	837	
1a,1b-dihomo-15-deoxy-delta-12,14-PGD2		C22 H34 O4	981	
1alpha,25-dihydroxy-11-(4-hydroxymethylphenyl)-9,11-didehydrovitamin D3 / 1alpha,25-dihydroxy-11-(4-		C34 H48 O4	623	
1alpha,25-dihydroxy-11-(4-hydroxymethylphenyl)-9,11-didehydrovitamin D3 / 1alpha,25-dihydroxy-11-(4-		C34 H48 O4	712	
1alpha-hydroxy-26,27-dinorvitamin D3 25-carboxylic acid / 1alpha-hydroxy-26,27-dinorcholecalciferol		C25 H38 O4	988	
26,26,26-trifluoro-25-hydroxy-27-norvitamin D3 / 26,26,26-trifluoro-25-hydroxy-27-norcholecalciferol		C26 H39 F3 O2	823	
2-Amino-3-methyl-1-butanol	473-75-6	C5 H13 N O	997	
2-amino-8-oxo-9,10-epoxy-decanoic acid		C10 H17 N O4	979	
4Z,7Z,10Z,13Z-eicosatetraenoic acid		C20 H32 O2	979	
5beta-Chola-8(14),11-dien-24-oic Acid		C24 H36 O2	917	
8alpha-3beta-hydroxy-estra-1,3,5(10)-trien-17-one	37242-41-4	C18 H22 O2	609	
Arachidonyl lysolecithin	63163-02-0	C28 H50 N O7 P	624	Geigy vol.3 p.121
C16 Sphinganine		C16 H35 N O2	984	
Cucurbitacin P		C30 H48 O7	962	
Docosanedioic acid		C22 H42 O4	833	
GlcNalpha1-6Ins-1-P-Cer(t18:0/26:0)		C56 H111 N2 O16 P	759	
Guanethidine	55-65-2	C10 H22 N4	965	Geigy Vol 4 Xenobiotics p.209
isoamyl nitrite		C5 H11 N O2	932	

Name	CAS	Formula	Similarity	Class
Methandrostenolone		C20 H28 O2	995	
Pantothenic Acid	137-08-6	C9 H17 N O5	979	Geigy vol.3 p.129
Purine	120-73-0	C5 H4 N4	991	
Purine	120-73-0	C5 H4 N4	1000	
Terbutaline		C12 H19 N O3	838	
Testosterone oxododecanoate	5874-98-6	C31 H48 O4	876	Androgen
Tiamulin	55297-95-5	C28 H47 N O4 S	394	Chemotherapeutic
Tiamulin	55297-95-5	C28 H47 N O4 S	616	Chemotherapeutic
Tiropramide	55837-29-1	C28 H41 N3 O3	616	Analgesic;Antispasmotic
Tocainide	41708-72-9	C11 H16 N2 O	951	Antiarrhythmic
trans-gondoic acid		C20 H38 O2	998	
Trp Ala Thr		C18 H24 N4 O5	969	
Uracil		C4 H4 N2 O2	852	
Not identified				
		C12 H21 N5 O	651	
		C42 H72 N4 O4	654	
		C10 H22 N4 O S	655	
		C10 H25 N3 O2 S	656	
		C9 H24 N4 O4	657	
		C9 H21 N3 O4	658	
		C5 H2 N2 O8 S	659	
		C5 H2 N2 O8 S	660	
		C5 H2 N2 O8 S	664	
		C5 H2 N2 O8 S	668	
		C13 H22 N2 S	668	
		C5 H2 N2 O8 S	673	
		C12 H2 N2 O3 S	675	
		C4 H5 N3 O4	677	
		C5 H2 N2 O8 S	682	
		C10 H29 N7 O	682	
		C12 H2 N2 O3 S	686	
		C12 H31 N5 O	694	
		C5 H2 N2 O8 S	695	
		C5 H2 N2 O8 S	696	

Name	CAS	Formula	Similarity	Class
		C9 H25 N7 O	701	
		C16 H N O4 S	704	
		C10 H27 N11	704	
		C5 H2 N2 O8 S	714	
		C5 H2 N2 O8 S	720	
		C10 H25 N7 O	722	
		C13 H22 N4 O3	724	
		C9 H18 N6 O2	726	
		C14 H9 N O4 S	727	
		C9 H21 N3 O4	728	
		C11 H27 N3 O5	731	
		C5 H4 O6	732	
		C12 H26 O7	734	
		C9 H14 N2 O8	736	
		C14 H8 O4 S	738	
		C11 H15 N7 O2	748	
		C11 H19 N7 O3	757	
		C36 H71 Cl N6 O4	758	
		C32 H71 Cl N6 O5	769	
		C9 H21 N3 O4	771	
		C34 H71 Cl N6 O5	773	
		C32 H69 Cl N12 O3	776	
		C38 H67 Cl N6 O5	779	
		C10 H29 N7 O	782	
		C38 H67 Cl N6 O5	785	
		C43 H69 Cl O2	787	
		C34 H69 Cl N6 O5	787	
		C5 H2 N2 O8 S	813	
		C5 H2 N2 O8 S	814	
		C12 H18 N4 O	819	
		C8 H23 N5 O4	843	
		C7 H6 N4 O5 S	843	
		C7 H6 N4 O5 S	847	
		C7 H6 N4 O5 S	848	

Name	CAS	Formula	Similarity	Class
		C7 H6 N4 O5 S	858	
		C7 H6 N4 O5 S	860	
		C7 H6 N4 O5 S	864	
		C7 H6 N4 O5 S	870	
		C7 H6 N4 O5 S	871	
		C43 H71 Cl O2	958	
		C40 H75 Cl O2 S	959	
		C36 H74 N10 O2 S	962	
		C37 H76 N10 O2 S	994	
		C15 H36 N4 O	780	
		C17 H32 N6 O3	977	
		C20 H24 N10 O5	973	
		C21 H40 N4 O3	984	
		C21 H44 N2 O9	430	
		C21 H45 N3 O5 S	923	
		C22 H37 N13 O5	871	
		C28 H27 N O30 S2	601	
		C29 H43 N5 O5	408	
		C31 H11 N11 O24	749	
		C31 H11 N11 O24	676	
		C31 H23 N O30 S	687	
		C35 H15 N5 O26	633	
		C39 H70 N26 S	977	
		C4 H5 N5 O	590	
		C5 H13 N O	848	
		C6 H2 N4 S3	733	
		C8 H20 N2 O3	978	
		C21 H47 N3 O5 S	930	
		C18 H43 N9 O3 S	947	
		C22 H32 N4 S	811	
		C16 H36 N18 O3 S	949	
		C21 H43 N13 O2 S	846	
		C19 H36 N18 O S	846	
		C19 H39 N13 S	488	

Name	CAS	Formula	Similarity	Class
		C29 H43 N5 S	847	
		C17 H41 N9 O9	944	
		C16 H39 N13 O5	964	
		C17 H43 N13 O5	942	
		C24 H43 N5 O5	816	
		C16 H41 N13 O4	757	
		C21 H35 N13 O2	717	
		C21 H41 N9 O4 S	705	
		C19 H35 N13 O5	956	
		C27 H39 N11 O3	681	
		C21 H45 N13 O2 S	773	
		C29 H41 N7 O2	771	
		C14 H38 N12 O8	935	
		C16 H38 N12 O8	382	
		C21 H45 N13 O2 S	826	
		C23 H35 N17 O	682	
		C14 H31 N17 O	964	
		C22 H38 N12 O3	717	
		C42 H86 N16 O10	989	
		C24 H45 N7 O4	891	
		C32 H6 N6 O18	944	
		C23 H49 N3 O5 S	911	
		C21 H41 N13 S	986	
		C25 H37 N3 O6	916	
		C17 H35 N13 O2	394	
		C36 H74 N16 O11	992	
		C19 H41 N15 O7	957	
		C25 H47 N9 O6	746	
		C40 H76 N20 O7	992	
		C22 H49 N5 O5 S	857	
		C25 H41 N11	787	
		C32 H6 N6 O18	934	
		C14 H42 N14 O5 S	881	
		C15 H42 N18 O S	740	

Name	CAS	Formula	Similarity	Class
		C24 H43 N13 S	958	
		C23 H41 N3 O5	951	
		C23 H51 N5 O8 S	850	
		C15 H37 N13 O5	399	
		C15 H42 N18 O S	716	
		C25 H47 N9 O4 S	973	
		C21 H45 N9 O3 S	944	
		C17 H46 N12 O2 S	426	
		C31 H37 N5	788	
		C24 H35 N7 O	829	
		C26 H47 N7 O4	889	
		C16 H39 N19 O3	951	
		C26 H45 N3 O5	784	
		C20 H41 N13 S	743	
		C30 H47 N5 S	791	
		C26 H37 N13	719	
		C19 H47 N13 O2 S	800	
		C30 H41 N9 O	682	
		C17 H43 N13 O5	911	
		C26 H39 N7 O	812	
		C23 H45 N O4	970	
		C26 H45 N13 S	963	
		C15 H42 N18 O S	791	
		C30 H47 N3 O5	749	
		C25 H41 N3 O5	806	
		C18 H46 N12 O3 S	838	
		C28 H47 N3 O5	773	
		C24 H45 N13 S	978	
		C33 H43 N5	356	
		C21 H47 N9 O4 S	476	
		C26 H43 N5	861	
		C30 H15 N7 O28	380	
		C28 H27 N O30 S2	607	
		C24 H55 N5 O3 S3	895	

Name	CAS	Formula	Similarity	Class
		C27 H57 N3 O S3	846	
		C24 H33 N13	781	
		C26 H47 N3 O3 S	775	
		C36 H78 N22 O9	494	
		C26 H49 N7 O4	868	
		C29 H49 N3 O6	940	
		C16 H43 N13 O2 S	759	
		C55 H82 N10 O5	785	
		C20 H43 N13 O5	890	
		C19 H49 N13 O2 S	804	
		C27 H45 N11	713	
		C20 H39 N19	778	
		C16 H33 N3 O	645	
		C32 H45 N O4	773	
		C25 H49 N O4	971	
		C32 H45 N9 O	796	
		C21 H51 N13 O2 S	860	
		C25 H45 N3 O5	982	
		C25 H43 N3 O5	800	
		C28 H51 Cl N8 O	476	
		C21 H47 N15 O2 S	940	
		C21 H51 N9 O3 S	926	
		C29 H45 N7 O	787	
		C27 H51 N7 O2 S	861	
		C23 H53 N5 O8 S	920	
		C18 H38 O4	991	
		C19 H47 N13 O5	962	
		C28 H47 N7 O2 S	863	
		C14 H30 N4 O3	680	
		C46 H68 N16 S	388	
		C44 H87 Cl2 N3 O3 S	409	
		C32 H70 N20 O S	355	
		C24 H49 N13 S	931	
		C22 H51 N13 O5	957	

Name	CAS	Formula	Similarity	Class
		C33 H53 N5 O5	803	
		C16 H39 N19 O3	969	
		C12 H28 N10 O	796	
		C44 H87 Cl2 N3 O3 S	412	
		C52 H72 N6 O6	401	
		C32 H67 N19 O S	321	
		C21 H47 N15 O S2	967	
		C29 H49 N11	866	
		C21 H52 N12 O3 S	831	
		C36 H51 N3 O3	721	
		C16 H39 N19 O3	962	
		C53 H68 N2 O	476	
		C44 H87 Cl2 N3 O3 S	415	
		C38 H83 N5 O S4	765	
		C34 H74 Cl N17 O4 S	730	
		C38 H72 N4 O5 S	865	
		C21 H49 N19 S	764	
		C22 H47 N19	704	
		C33 H60 N4 O9	979	
		C35 H55 N3 O9	492	
		C35 H57 N3 O3 S	762	
		C18 H43 N19 O3	966	
		C37 H77 N15 O3 S3	875	
		C16 H39 N19 O3	959	
		C37 H79 Cl2 N13 O2	428	
		C43 H72 Cl N9 O3	631	
		C32 H60 N18	810	
		C46 H73 N7 O8	633	
		C38 H83 N5 O S4	765	
		C36 H77 Cl2 N13 O2 S	616	
		C34 H75 N11 O9	617	
		C53 H78 Cl N O7	871	
		C45 H90 Cl N O2 S3	367	

Name	CAS	Formula	Similarity	Class
		C36 H79 N7 O3 S3	805	
		C38 H72 Cl N11 O5	808	
		C57 H71 N S	806	
		C35 H69 N15 O8	644	
		C41 H86 Cl N7 S3	775	
		C39 H83 N3 O2 S4	777	
		C49 H75 N3 O2 S2	848	
		C40 H85 N5 O4 S4	686	

Herring gull GC-MS

Name	CAS	Fomula	Similarity	Class	ng/sample
OP					
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	C9 H18 Cl3 O4 P	872	OP	78
Ethanol, 2-butoxy-, phosphate (3:1)	78-51-3	C18 H39 O7 P	797	OP	28
Tri(2-chloroethyl) phosphate	115-96-8	C6 H12 Cl3 O4 P	748	OP	10
1-Propanol, 2,3-dichloro-, phosphate (3:1)	78-43-3	C9 H15 Cl6 O4 P	703	OP	7,9
Tributyl phosphate	126-73-8	C12 H27 O4 P	790	OP	6,1
Triphenyl phosphate	115-86-6	C18 H15 O4 P	769	OP	2,6
Other polymer components/additives					
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4	C14 H22 O	892	Antioxidant	77
2(3H)-Benzothiazolone	934-34-9	C7 H5 N O S	855	Benzothiazole	52
3,5-di-tert-Butyl-4-hydroxyacetophenone	14035-33-7	C16 H24 O2	775	Antioxidant	25
Bayer 28,589	728-40-5	C14 H21 N O3	766	Antioxidant	10
Butylated Hydroxytoluene	128-37-0	C15 H24 O	825	Antioxidant	8,1
Halogenated compounds/ Pesticides					
1,1'-Biphenyl, 2,2',3,5'-tetrachloro-		C12 H6 Cl4	718	PCB	172
2,2',3,4',5,6'-Hexachloro-1,1'-biphenyl		C12 H4 Cl6	907	PCB	168
p,p'-DDE	72-55-9	C14 H8 Cl4	931	Pesticide	128
2,2',3,4',5,6'-Hexachloro-1,1'-biphenyl		C12 H4 Cl6	918	PCB	71
1,1'-Biphenyl, 2,4,4'-trichloro-		C12 H7 Cl3	729	PCB	44
2,3,3',4',5-Pentachloro-1,1'-biphenyl		C12 H5 Cl5	844	PCB	43
1,1'-Biphenyl, 2,2',3,4,4',5,6'-Heptachloro-		C12 H3 Cl7	777	PCB	40
1,1'-Biphenyl, 2,2',3',4,5-Pentachloro-		C12 H5 Cl5	837	PCB	39
Oxychlordan	27304-13-8	C10 H4 Cl8 O	714	Pesticide	37
1,1'-Biphenyl, 2,2',3,3',4,5'-hexachloro-		C12 H4 Cl6	824	PCB	35
trans-Nonachlor		C10 H5 Cl9	782	Pesticide	33
Photo-Mirex	53308-47-7	C10 H Cl11	782	Pesticide	32
1,1'-Biphenyl, 2,2',3,3',4,5,5'-heptachloro-		C12 H3 Cl7	851	PCB	29
1,1'-Biphenyl, 2,3',4,5,5'-pentachloro-		C12 H5 Cl5	818	PCB	29

Name	CAS	Fomula	Similarity	Class	ng/sample
Dieldrin	60-57-1	C12 H8 Cl6 O	746	Pesticide	27
Toxaphen	8022-04-6	C10 H10 Cl8 (average)	833	Pesticide	20
trans-Nonachlor		C10 H5 Cl9	711	Pesticide	18
1,1'-Biphenyl, 2,3,3',4,6-Pentachloro-		C12 H5 Cl5	704	PCB	17
cis-Nonachlor		C10 H5 Cl9	788	Pesticide	15
1,1'-Biphenyl, 2,3',4,6-Tetrachloro-		C12 H6 Cl4	791	PCB	14
1,1'-Biphenyl, 2,2',3,3',4,5,5'-heptachloro-		C12 H3 Cl7	812	PCB	14
1,1'-Biphenyl, 2,3',4,4'-tetrachloro-		C12 H6 Cl4	731	PCB	12
2,2',3,4,5,6-Hexachloro-1,1'-biphenyl		C12 H4 Cl6	793	PCB	11
1,1'-Biphenyl, 2,2',3,3',4,5',6'-heptachloro-		C12 H3 Cl7	818	PCB	11
1,1'-Biphenyl, 2,2',3,3',4,5,5'-heptachloro-		C12 H3 Cl7	830	PCB	9,9
2,2',3,4',5,6'-Hexachloro-1,1'-biphenyl		C12 H4 Cl6	865	PCB	9,7
Heptachlor epoxide	1024-57-3	C10 H5 Cl7 O	753	Pesticide	8,1
DDMU	1022-22-6	C14 H9 Cl3	750	Pesticide	7,7
2,3',4,4',5'-Pentachloro-1,1'-biphenyl		C12 H5 Cl5	792	PCB	7,5
Chlordane	57-74-9	C10 H6 Cl8	756	Pesticide	6,9
1,1'-Biphenyl, 2,3',4,6-Tetrachloro-		C12 H6 Cl4	752	PCB	6,2
2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1	C12 H6 OBr4	723	PBDE	5,9
1,1'-Biphenyl, 2,3,3',4,5,6-hexachloro-		C12 H4 Cl6	765	PCB	5,8
1,1'-Biphenyl, 2,2',3,3',4,5'-hexachloro-		C12 H4 Cl6	705	PCB	4,8
Mirex	2385-85-5	C10 Cl12	791	Pesticide	4,4
1,1'-Biphenyl, 2,2',3',4,5-Pentachloro-		C12 H5 Cl5	823	PCB	3,7
1,1'-Biphenyl, 2,2',4,6-Tetrachloro-		C12 H6 Cl4	818	PCB	3,3
1,1'-Biphenyl, 2,2',3,3',6-pentachloro-		C12 H5 Cl5	720	PCB	2,3
1,1'-Biphenyl, 2,2',3,3',5,5',6-heptachloro-		C12 H3 Cl7	791	PCB	1,2
1,1'-Biphenyl, 2,3,3',4,4',5'-hexachloro-		C12 H4 Cl6	749	PCB	0,9
2,2',4,4',6-Pentabromodiphenyl ether		C12 H5 OBr5	760	PBDE	0,8
PAC					
Pyrene	129-00-0	C16 H10	852	PAH	11
Fluoranthene	206-44-0	C16 H10	875	PAH	9,3

Herring gull LC-MS

Name	CAS	Fomula	Similarity	Class
Biocides				
Atrazine-desethyl	6190-65-4	C6 H10 Cl N5	684	herbicide
Rubijervine	79-58-3	C27 H43 N O2	966	Fungicide
Phthalates				
diethyl phthalate		C12 H14 O4	888	phthalate
OPs				
Ethanol, 2-butoxy-, phosphate (3:1)		C18 H39 O7 P	798	OP
Pharmaceuticals and biomolecules				
Amiflamine	77518-07-1	C12 H20 N2	984	MAO inhibitor
Anagestone	2740-52-5	C22 H34 O2	994	Progestin
Androstendiol dipropionate	2297-30-5	C25 H38 O4	975	Anabolic
Bornelone	119-37-5	C14 H20 O	954	
Buprenorphine	52485-79-7	C29 H41 N O4	794	Opioid
Carpindolol	39731-05-0	C19 H28 N2 O4	666	Beta-Blocker
Cholestenone	601-57-0	C27 H44 O	857	Biomolecule
Ciclactate	15145-14-9	C12 H22 O3	823	Antispamotic
Citrulline	372-75-8	C6 H13 N3 O3	877	LiverProtective
Cyclobenzaprine	303-53-7	C20 H21 N	682	Neuroleptic
Delanterone	63014-96-0	C20 H28 O	950	Antiandrogen
Desmethylmoramide	1767-88-0	C24 H30 N2 O2	710	Analgesic
Devapamil	92302-55-1	C26 H36 N2 O3	707	CaAntagonist
Dimemorfan	36309-01-0	C18 H25 N	751	Antitussive
Dimethylaminoethyl- nicotinamidobenzoate		C17 H19 N3 O3	940	LocalAnesthetic
Dimethylandrostanolone	2881-21-2	C21 H34 O2	853	Anabolic
Drostanolone	58-19-5	C20 H32 O2	965	Anabolic
Eikosapentaenic acid		C20 H32 O2	856	Choleretic
Ephedrine-D3	299-42-3	C10 H12 D3 N O	878	Sympathomimetic
Etaminil	15599-27-6	C15 H22 N2	697	Antitussive
Fenoxypropazine	3818-37-9	C9 H14 N2 O	854	Antidepressant
Fexofenadine	83799-24-0	C32 H39 N O4	755	antihistaminic

Name	CAS	Fomula	Similarity	Class
Gaboxadol		C6 H8 N2 O2	696	Analgesic
Geroquinol	10457-66-6	C16 H22 O2	749	RadiationProtectant
Medetomidine	86347-14-0	C13 H16 N2	757	Sedative
Meladrazine	13957-36-3	C11 H23 N7	672	Muscle relaxant
Mexenone	1641-17-4	C15 H14 O3	850	Dermatic
Nabilone	51022-71-0	C24 H36 O3	988	Tranquilizer
Octacaine	13912-77-1	C14 H22 N2 O	703	LocalAnesthetic
Orestrate	13885-31-9	C27 H36 O3	652	Estrogen
Pentylurea	38869-91-9	C6 H14 N2 O	765	Sedative
Pimetine	608-19-4	C16 H26 N2	797	Anticholesteremic
Promestriene	39219-28-8	C22 H32 O2	781	Corticoid
PYCC	22912-25-0	C11 H18 N2	952	Psychedelic;DesignerDrug
Quinisocain	86-80-6	C17 H24 N2 O	780	LocalAnesthetic
Terbutaline		C12 H19 N O3	950	
Tocainide	41708-72-9	C11 H16 N2 O	677	Antiarrhythmic
Not identified			**0**	
		C16 H28 O5	651	
		C5 H2 N2 O8 S	652	
		C36 H61 N O5	653	
		C4 H2 S	654	
		C31 H69 N17 O8	654	
		C5 H2 N2 O8 S	655	
		C6 H14 O9 S	658	
		C27 H56 Cl2 N4 O6	658	
		C41 H67 N11 O	660	
		C46 H81 N3 O2 S4	670	
		C28 H50 Cl2 N2 O2	671	
		C24 H47 Cl N4 O3 S	674	
		C9 H14 N6 O4	674	
		C43 H76 N4 O2	675	
		C12 H36 N14 O4	677	
		C10 H25 N7 O	678	
		C46 H67 Cl O3	684	
		C12 H31 N7 O	685	

Name	CAS	Fomula	Similarity	Class
		C6 H2 O12	686	
		C52 H67 N3 O2	688	
		C42 H74 N4 O2	693	
		C21 H35 Cl N4	694	
		C24 H52 Cl2 N4 O5	706	
		C4 H2 S	707	
		C29 H52 O7	708	
		C18 H36 O2	712	
		C27 H56 Cl2 N4 O6	712	
		C5 H2 N2 O8 S	725	
		C44 H84 O S2	729	
		C5 H2 N2 O8 S	730	
		C12 H Cl O3 S	737	
		C10 H11 N7 O3	737	
		C5 H2 N2 O8 S	745	
		C14 H24 O3 S	747	
		C34 H50 N4 O4	747	
		C27 H46 N10 O	749	
		C9 H14 N2 O8	750	
		C33 H49 N3 O S	764	
		C41 H65 Cl N10 O	767	
		C41 H65 Cl N10 O	774	
		C28 H42 N4	776	
		C38 H67 Cl N6 O5	779	
		C39 H80 O3 S4	779	
		C44 H78 O S	783	
		C23 H34 N6	784	
		C29 H52 O5	787	
		C31 H24 Cl N O30 S	789	
		C22 H42 O3	790	
		C12 H3 N3 O3 S	798	
		C31 H24 Cl N O30 S	798	
		C40 H76 O S2	801	
		C5 H2 N2 O8 S	801	

Name	CAS	Fomula	Similarity	Class
		C26 H43 N O2	803	
		C18 H34 O2	805	
		C44 H73 N7 O2	823	
		C8 H12 O3 S	832	
		C18 H34 O2	833	
		C20 H36 O2	834	
		C7 H4 O5 S3	834	
		C12 H14 N10	835	
		C20 H36 O2	839	
		C20 H38 O3	840	
		C18 H34 O2	842	
		C7 H6 N4 O5 S	846	
		C7 H6 N4 O5 S	852	
		C18 H34 O2	857	
		C18 H32 O2	859	
		C8 H12 O3 S	860	
		C8 H12 O3 S	861	
		C7 H6 N4 O5 S	868	
		C30 H64 N2 S4	874	
		C5 H4 N4	876	
		C25 H46 O7	886	
		C38 H74 N4 O4 S	896	
		C20 H38 O2	898	
		C7 H3 Cl N2 O5	898	
		C26 H39 Cl N4	900	
		C50 H81 N7 O S3	902	
		C24 H48 N2 O5	909	
		C8 H2 N4 O6 S	910	
		C16 H34 N6	915	
		C39 H76 N4 O4 S	915	
		C43 H73 N11 S2	915	
		C49 H77 N O3 S3	926	
		C34 H74 N10 S	936	
		C24 H39 Cl N4	948	

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		C20 H43 N7 O S	961	
		C30 H56 S2	962	
		C26 H52 O2	970	
		C22 H38 O2	972	
		C30 H58 O4	977	
		C26 H52 O2	981	
		C17 H34 O2	984	
		C22 H43 N O3	984	
		C39 H68 N4 O2	984	
		C33 H61 N5 O S	985	
		C17 H34 O2	986	
		C17 H32 O2	986	
		C18 H38 N2 O7	990	
		C19 H36 O2	994	
		C16 H33 N3 O	656	
		C21 H43 N11 O6	660	
		C17 H44 N12 O8	665	
		C42 H71 N9 O4	668	
		C24 H48 S	677	
		C21 H35 N17 O	686	
		C22 H41 N13 O5	688	
		C35 H65 N23	690	
		C44 H91 N O3 S4	691	
		C38 H82 N6 O2 S3	691	
		C21 H48 Cl N5 O7	695	
		C29 H65 N25 O2	696	
		C38 H82 N6 O2 S3	701	
		C34 H69 N19 O4	701	
		C27 H61 N27 O	704	
		C31 H65 N21 O3	710	
		C31 H65 N21 O3	712	
		C10 H5 N O	716	
		C16 H35 N19 S	718	
		C32 H67 N5	723	

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		C45 H90 Cl N O2 S3	725	
		C30 H65 N9 O	726	
		C45 H77 N5 O S2	732	
		C42 H85 N O5 S3	734	
		C20 H41 N13 O5	737	
		C19 H45 N13 O5	737	
		C20 H43 N9 O	744	
		C26 H42 O S	746	
		C17 H47 N19 S	746	
		C32 H43 N3 O6	749	
		C23 H42 N8 O7	751	
		C17 H43 N19 S	757	
		C31 H11 N11 O24	758	
		C15 H36 N4 O	759	
		C26 H40 N6 O3	759	
		C46 H82 N22 O S	762	
		C32 H43 N3 O6	762	
		C33 H39 N7 O2	764	
		C30 H45 N7 O2	764	
		C19 H43 N19 S	766	
		C45 H75 N5 O6	766	
		C28 H59 N3 O3 S2	768	
		C18 H37 N19 O3	769	
		C30 H15 N7 O28	770	
		C20 H41 N13 O2	771	
		C38 H52 O2 S	773	
		C36 H55 N3 O3	774	
		C21 H N O18 S	780	
		C18 H41 N17 O3	780	
		C17 H43 N15 O7	781	
		C22 H51 N13 O5	783	
		C17 H43 N19 S	784	
		C22 H45 N13 O2	785	

Name	CAS	Fomula	Similarity	Class
		C28 H51 N3 O3 S2	786	
		C38 H82 Cl N11 O S2	791	
		C21 H49 N19 S	792	
		C31 H39 N3 O3	793	
		C34 H39 N9 O	793	
		C33 H53 N5 O5	796	
		C32 H49 N O9	796	
		C14 H42 N14 O5 S	797	
		C29 H49 N5 O5	800	
		C18 H48 N14 O5 S	801	
		C44 H75 N5 O S2	802	
		C25 H47 N S2	802	
		C16 H33 N17 O	804	
		C25 H43 N11 O3	805	
		C26 H39 N7 O	808	
		C48 H73 N5 O S	810	
		C13 H16 N6	810	
		C25 H49 N O4	812	
		C39 H68 N10 O3	813	
		C19 H38 N4 S	813	
		C20 H N O23	817	
		C4 H12 N4 O	818	
		C16 H37 N21	818	
		C26 H37 N5	818	
		C21 H51 N13 O2 S	820	
		C32 H51 N O4 S	820	
		C21 H48 N12 O3 S	821	
		C35 H47 N3 O S	823	
		C8 H8 O	824	
		C21 H38 N4 S	827	
		C48 H86 Cl N O2 S2	827	
		C23 H43 N O2	830	
		C20 H N O23	831	

Name	CAS	Fomula	Similarity	Class
		C9 H22 N4 O3	833	
		C19 H33 N9 O	839	
		C39 H68 N10 O3	845	
		C42 H76 O9	845	
		C20 H50 N8 O7 S	845	
		C19 H38 N4 S	848	
		C8 H10 N2 O2	848	
		C5 H14 N2	849	
		C12 H15 N S	850	
		C17 H34 O2 S	852	
		C10 H24 N2 O3	852	
		C17 H33 N9 O	853	
		C21 H38 N4 S	854	
		C19 H48 N12 O3 S	854	
		C24 H45 N7 O4	855	
		C37 H79 Cl2 N13 O2	859	
		C25 H53 N13 O2 S	860	
		C19 H40 N4 S	862	
		C40 H85 N3 O2 S4	862	
		C43 H79 N O5 S2	862	
		C20 H46 N8 O7 S	863	
		C19 H45 N13 O2 S	864	
		C33 H33 N5	865	
		C19 H45 N13 O2 S	865	
		C31 H49 N O4 S2	866	
		C14 H38 N12 O8	867	
		C24 H53 N3 O8 S	870	
		C29 H51 N3 O8	871	
		C39 H75 N7 O3 S2	871	
		C23 H41 N17 O	871	
		C30 H47 N7 O2 S	877	
		C45 H73 N5 O S	880	
		C22 H45 N3 O5 S	881	
		C44 H81 N O5 S2	883	

Name	CAS	Fomula	Similarity	Class
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		C22 H40 O3 S	889	
		C23 H47 N17 O	889	
		C14 H39 N9 O9	894	
		C50 H75 N S2	895	
		C51 H69 N5 O	896	
		C50 H75 N S2	897	
		C16 H35 N17 O	902	
		C16 H41 N19 O3	908	
		C26 H45 N3 O6 S	909	
		C20 H43 N13 O5	909	
		C17 H34 N18 O3	913	
		C26 H51 N5 O8 S	915	
		C23 H47 N3 O6 S	918	
		C17 H41 N13 O5	922	
		C19 H45 N11 O6	922	
		C26 H36 N4	923	
		C19 H37 N13 S	924	
		C24 H32 N4	929	
		C22 H34 N16 O5	930	
		C23 H45 N5 O2	930	
		C25 H41 N O2	931	
		C8 H10 N2 O2	932	
		C27 H39 N7	932	
		C27 H39 N7 O2	933	
		C21 H43 N13 S	938	
		C21 H45 N11 O	938	
		C8 H16 N8 O S	938	
		C19 H42 N18 O S	939	
		C17 H35 N13 S	941	
		C20 H39 N13 S	945	
		C34 H70 O8 S	945	
		C23 H45 N13 S	949	
		C25 H40 N12 O5 S	950	

Name	CAS	Fomula	Similarity	Class
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		C26 H36 N4	952	
		C19 H49 N11 O6 S2	955	
		C16 H39 N19 O3	957	
		C28 H50 N10 O6	958	
		C18 H38 O4	961	
		C21 H43 N13 S	961	
		C22 H50 N10 O6	965	
		C25 H40 N12 O5 S	966	
		C32 H50 O6	967	
		C8 H21 N3	968	
		C25 H48 O9 S	968	
		C23 H45 N O4	969	
		C32 H60 N12 O2	971	
		C21 H38 O3	971	
		C38 H79 N5 O9 S	972	
		C21 H47 N9 O9	976	
		C23 H36 O4	977	
		C48 H80 O10	978	
		C35 H55 N3 O9	979	
		C25 H47 N O4	979	
		C27 H51 N O4	980	
		C22 H51 N13 O5	980	
		C21 H38 N4 O	981	
		C17 H28 O9	982	
		C25 H50 N10 O6	983	
		C22 H44 N6 O5	984	
		C12 H20 O4	991	
		C16 H41 N19 O3	992	
		C19 H36 O4	994	
		C43 H82 N20 O7	995	
		C31 H57 N5 O11	996	

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Forfatter(e) Martin Schlabach, Peter Haglund, Pawel Rostkowski and Christian Dye

Tittel - norsk og engelsk Non-target screening - A powerful tool for selecting environmental pollutants Ikke spesifikk screening – Et kraftfull redskap for utvelgelse av miljøgifter

Sammendrag – summary The main goal with this project was to test the potential and practicalness of the available non-target screening methods for identification of unknown or new emerging environmental pollutants. It was also desired to try to estimate the quantity of the identified compounds.

4 emneord Nye stoffer, non-target screening, miljøgifter, PPCPer	4 subject words Emerging contaminants, non-target screening, environmental pollutants, PPCPs

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Statlig program for forurensningsovervåking omfatter overvåking av forurensningsforholdene i luft og nedbør, skog, vassdrag, fjorder og havområder.

Overvåkingsprogrammet dekker langsiktige undersøkelser av:
•overgjødsling•forsuring (sur nedbør)
•ozon (ved bakken og i stratosfæren)
•klimagasser
•miljøgifter

Overvåkingsprogrammet skal gi informasjon om tilstanden og utviklingen av forurensningssituasjonen, og påvise eventuell uheldig utvikling på et tidlig tidspunkt. Programmet skal dekke myndighetenes informasjonsbehov om forurensningsforholdene, registrere virkningen av iverksatte tiltak for å redusere forurensningen, og danne grunnlag for vurdering av nye tiltak. Miljødirektoratet er ansvarlig for gjennomføringen av overvåkingsprogrammet.