Nordic Council of Ministers

Maximizing output from non-target screening

Contents

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1 Introduction

1.1 Project background

In recent years, there has been a paradigm shift in chemical analysis, which has been possible with the introduction of chromatography in combination with high-resolution accurate mass spectrometry (for example QTOF or Orbitrap). This means that the analyzes can to a greater extent be used to detect new chemicals in, for example, environmental samples, without having decided in advance what to look for. This opens up a field with extreme potential in relation to environmental monitoring and in extension of this also in relation to the possibility of starting the regulation process for new substances that constitute a potential health and/or environmental hazard.

Under the Nordic Screening Group (www.nordicscreening.org), and with support from the Nordic Chemical Group (NKG) and the Nordic Marine Group (HAV), a suspect screening analysis was performed in 2015 and 2016, which was based precisely on such sophisticated analysis methods just mentioned. The results were published by Schlabach and co-workers in the TemaNord 2017:561 report (Schlabach et al. 2017).

By using these advanced chemical analyzes methods, a large amount of data is generated, as was the case for the Nordic Screening project (Schlabach et al. 2017). However, the interpretation possibilities of this data are currently limited by databases that have largely been institution-specific, in addition to often being instrument-specific by proprietary software, and of course by the availability of resources in the form of man-hours. There is a great deal of work involved in interpreting analysis data in relation to which chemical substances they represent, and this is the background for this current project. There is a wealth of data on chemical substances in the Nordic samples – but it has only been possible to unambiguously identify a small part of these. Another need in relation to optimal use of this data is the need of a description of the identified substance in relation to whether it is a natural or an anthropogenic from the technosphere.

1.2 Project aim and method

The purpose of this project is to optimize the benefits of the major work that has already been done with careful sample selection and sampling in all of the Nordic countries, with meticulous sample preparation and chemical analysis by a consortium of some of the Nordic region's most experienced scientific groups in analyses of emerging environmental contaminants. But where perhaps the full potential of the generated data is still to be realized. This project will dig deeper into the data material and try to further identify and describe the substances already detected, to be able to better understand what substances we in modern Nordic societies release into the sea via our wastewater.

The work was divided into the following tasks:

- Semi-quantification of the compounds already identified
- Identify more of the compounds via suspect lists and quarry the digital archive files

Because this project mainly consists of data analysis and data curation of list by matching to different types of databases, the results are mainly presented as data tables. Thus, this report can be viewed as a data appendix to the initial report by Schlabach et al. (2017).

Further, all the data presented in this report are available on GitHub (https://github.com/umhvorvisstovan/NKG_Maximising_output_from_non_target_screening).

The analysis and identification of compounds in the environmental matrices may be described as a tiered approach as described by Schymanski et al. (2015). In this approach the identification is classified to a levels degree, where the results of non-target screening may be ranked from low confidence data (Level 5) to high confidence data (Level 1), where Level 1 and 2 corresponds to the confidence level normally aspired to in standard monitoring analysis of environmental contaminants. The knowledge gained at the various levels corresponds to:

Level 1: confirmed structure of the molecule (based on reference standard)

Level 2: a probable structure (based in library/diagnostic evidence)

Level 3: a tentative candidate compound

Level 4: an unequivocal molecular formula (but insufficient evidence of structure)

Level 5: a (molecular/ion) mass

In the present work, the aim has been to identify as many compounds as possible to Level 1, 2 and 3.

1.3 Sampling

Figure 1.1 depicts the sampling stations, samples were collected in the fall of 2015 in Greenland (GL), Iceland (IS), Faroe Islands (FO), Norway (NO), Denmark (DK), Sweden (SE), and Finland (FI). Further information on each sample can be found in Table 5.1 in Appendix 5 and in the initial study (Schlabach et al. 2017).

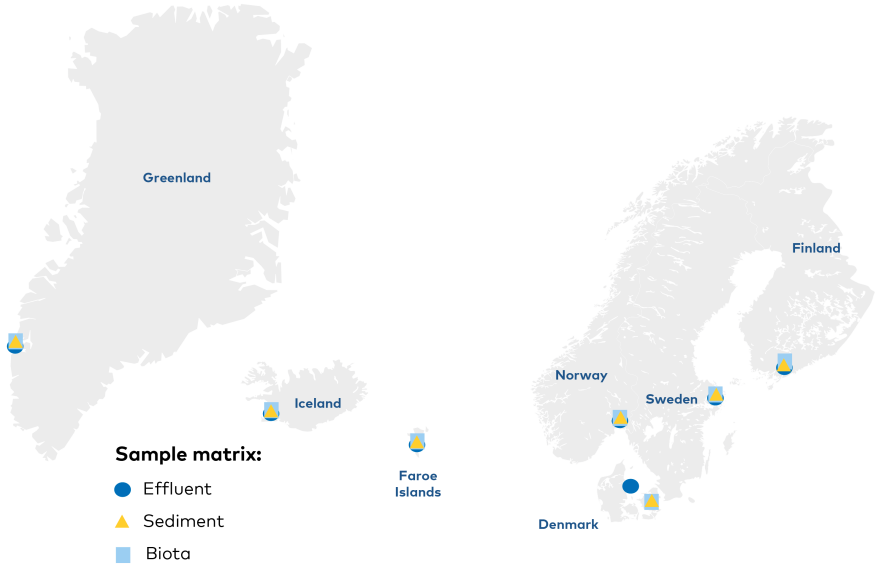

Figure 1.1 Sampling stations

2 Semi-quantification of the compounds already identified

2.1 Aim

The compounds detected by the GCxGC-MS (in biota) will be quantified to the extent possible (without internal standards per se, i.e., crude estimate from peak area).

2.2 Method

First estimation A first semi-quantification was performed based on area ratios of the most abundant ions in GC-MS spectra (the base peak) of sample components and internal standards. The internal standards were added in known amounts and the concentration of the biota contaminants were obtained by multiplying this quantity by the area ratio and dividing by the sample weight.

Methodology improvement However, often the contaminants were fragmenting more in the GC-MS instrument than the internal standards, leading to an underestimation of the concentrations.

Therefore, new calculations have been performed using a correction factor, see Equation (2.1)

$$Correction\ \ factor = \frac{(Total\ \ area\ \ of\ \ all\ \ ions\ \ /\ \ Area\ \ of\ \ base\ \ peak\ \ ion)_{sample}}{(Total\ \ area\ \ of\ \ all\ \ ions\ \ /\ \ Area\ \ of\ \ base\ \ peak\ \ ion)_{internal\ \ standard}} \qquad (2.1)$$

The corrected concentrations were then obtained by multiplying the first concentration estimates by the correction factor.

2.3 Results of semi-quantification of biota samples

The results of the refined estimate of the concentration of the substances which previously had been analyzed using semi-quantitative methods and were identified to the level 2 and 3 (Schlabach et al. 2017), are shown in Table 2.1. The refined estimate is based on correction factors as described in the Methods section. The correction factor and new concentration estimates for each sample are given in Table 2.1. The refined estimate is based on correction factors which range between 0.8 and 6.7, with an average of 2.1. Thus, the new concentrations are generally twice as high as the previous concentrations. Larger deviations were mainly observed for fragile molecules, such as fatty acids, fatty acid methyl esters, hydrocarbons, and long-chain aldehydes. However, also PCBs had previously been underestimated due to their abundant natural isotope ion distribution clusters.

Table 2.1 Results of the improved methodology in semi-quantification of the GC-MS detected compounds in the biota samples

Molecular Formula	Name	CAS	Norman SusDat ID	Corr. Factor	GL	IS	FO	NO	DK	SE	FI
					New concentration (ng/g)						
C8H12O	(E,E)-3,5-Octadien-2-one	30086-02-3		1.90	310	163.0	308	618.0	1,320.0	1,324	1,118.0
C10H22O3	1-(2-Butoxy-1-methylethoxy) propan-2-ol	29911-28-2	NS00002704	1.10					4.0		
C9H10O3	1-(2,4-Dihydroxy-3-methylphenyl) ethanone	10139-84-1		1.00		7.6		36.0			
C9H10O3	1-(2,4-Dihydroxy-3-methylphenyl) ethanone	10139-84-1		0.95					42.0		
C9H10O3	1-(2,4-Dihydroxy-3-methylphenyl) ethanone	10139-84-1		0.98						187	88.0
C14H14	1,1'-Biphenyl, 2,3'-dimethyl-	611-43-8		2.20					82.0	94	52.0
C14H14	1,1'-Biphenyl, 2,4'-dimethyl-	611-61-0		2.00					34.0	38	25.0
C7H5NS	1,2-Benzisothiazole	272-16-2		1.20	1,570		48	555.0			
C13H16	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6	NS00022016	1.80	179					11	4.8
C13H18	1,2,3,4-Tetrahydro-1,6,8-trimethylnaphthalene	30316-36-0		1.20	76						
C7H8O2	1,3-Benzenediol, 5-methyl-	504-15-4	NS00032059	1.40					52.0	18	
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	3.30	445		1,067	1,779.0			
C23H40O3	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	71041-49-1		1.30	219	9,103.0		2,131.0	1,330.0	765	408.0
C21H36O3	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	86879-46-1		1.10	54	1,596.0		465.0		115	67.0
C21H36O3	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	86879-46-1		1.00					646.0		
C9H8O1	1H-Inden-1-one, 2,3-dihydro-	83-33-0	NS00038249	1.90					80.0	91	
C8H7N1S2	2-(Methylthio)benzothiazole	615-22-5	NS00007832	2.30				24.0	72.0	60	
C16H34O3	2-[2-(Dodecyloxy) ethoxy]ethanol	3055-93-4	NS00013814	3.20	1,653						
C12H22	2-Ethyldecahydronaphthalene, (Z,E)-	66660-41-1		2.10		2,192.0	50				
C9H8O3	2-Hydroxy-5-methylisophthalaldehyde	7310-95-4	NS00037473	1.60						12	
C7H5N1S2	2-Mercaptobenzothiazole	149-30-4	NS00000568	1.10				461.0			
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	1.40					4.6		
C8H10O2	2-Phenoxyethanol	122-99-6	NS00002984	1.50							8.7
C9H8O	2-Phenylpropenal	4432-63-7	NS00076572	1.50	15	30.0		41.0	4.9		
C11H16O2	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	17092-92-1		2.10	242	55.0					
C11H16O2	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	17092-92-1		2.00					104.0		
C14H8N2S2	2,2'-Bibenzothiazole	4271-09-4		1.30					37.0		
C12H3Cl7	2,2',3,3',4,4',5-Heptachloro-1,1'-biphenyl (PCB 170)	35065-30-6	NS00114249	3.30				69.0			7.4
C12H5Cl5	2,2',3,4,6-Pentachlorobiphenyl	55215-17-3		3.60				78.0		26	17.0

Molecular Formula	Name	CAS	Norman SusDat ID	Corr. Factor	GL	IS	FO	NO	DK	SE	FI
					New concentration (ng/g)						
C12H6Cl4	2,2',5,5'-Tetrachlorobiphenyl (PCB 52)	35693-99-3	NS00001956	2.10	100	180.0	175	79.0	61.0	35	33.0
C15H28	2,2,4,4,7,7-Hexamethyloctahydro-1H-indene	54832-83-6		7.00		2,144.0	436				
C12H5Cl5	2,3',4,4',5-Pentachlorobiphenyl (PCB 118)	31508-00-6	NS00001962	3.60				186.0			
C12H4Cl6	2,3',4,4',5,5'-Hexachlorobiphenyl (PCB 167)	52663-72-6	NS00099486	3.30				254.0			21.0
C12H22	2,3-Dimethyldecahydronaphthalene	1008-80-6		2.60		46,944.0	87				
C12H5Cl5	2,3,3',4,4'-Pentachlorobiphenyl (PCB 105)	32598-14-4	NS00114177	2.20		103.0		101.0			
C12H4Cl6	2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8		3.70		308.0		612.0		22	29.0
C16H20	2,6-Diisopropylnaphthalene	24157-81-1	NS00010761	2.30		105.0					11.0
C9H12O2	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	NS00010663	1.50	11				21.0	309	153.0
C13H20O	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	NS00075791	1.80	415	178.0		210.0	347.0		
C12H24O3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3		2.10	68	132.0	111	118.0	83.0	49	67.0
C7H7NO2	3-Methyl-2-vinylmaleimide	21494-57-5		1.30					13.0		
C8H16O	3,4-dimethylcyclohexan-1-ol	5715-23-1	NS00046141	2.80	1,250	223.0	94	422.0	548.0	75	
C8H10O1	4-Ethylphenol	123-07-9	NS00010739	1.00				7.9			
C14H14	4,4'-Dimethylbiphenyl	613-33-2	NS00034646	2.00					21.0	23	17.0
C6H8O3	5-acetyldihydrofuran-2(3H)-one	29393-32-6	NS00049070	1.00					10.0	56	17.0
C14H26O2	9-Tetradecenoic acid, (9Z)-	544-64-9	NS00020426	6.70	22,039	24,996.0		23,201.0	20,693.0	22,395	11,211.0
C17H28	BENZENE, (1-BUTYLHEPTYL)-	4537-15-9	NS00095862	1.20		1,530.0	58				
C18H30	BENZENE, (1-PENTYLHEPTYL)-	2719-62-2	NS00008712	1.30		1,056.0	152				
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		0.79				83.0			
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		0.80						100	74.0
C15H13N1	Benzenepropanenitrile, .beta.-phenyl-	61310-06-3	NS00010691	1.10				54.0			
C7H6O2	Benzoic acid	65-85-0	NS00008785	2.00	272	116.0	180	1,100.0	88.0	293	212.0
C20H32O2	Benzoic acid, tridecyl ester		NS00076546	1.70							8.3
C13H10O1	Benzophenone	119-61-9	NS00010632	1.50		40.0					
C7H5N1S1	Benzothiazole	95-16-9	NS00000291	1.20			374	2,234.0	495.0	300	216.0
C7H5N1O1S1	Benzothiazolone	934-34-9	NS00008199	1.70	101				89.0	23	
C9H10O2	Benzyl acetate	140-11-4	NS00002107	2.30				91.0	170.0		171.0
C13H20O1	beta-Ionone	79-77-6	NS00001727	2.40	346						
C15H24	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9		5.20	15	1,284.0	135				
C8H10N4O2	Caffeine	58-08-2	NS00000273	1.80			80				
C18H26O1	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	1222-05-5	NS00008760	1.80		108.0	196	217.0		77	
C11H20	Decahydro-2-methylnaphthalene	2958-76-1	NS00096217	3.00		11,251.0	277				
C8H8O2	Ethanone, 2-hydroxy-1-phenyl-	582-24-1	NS00022418	1.40						12	

Molecular Formula	Name	CAS	Norman SusDat ID	Corr. Factor	GL	IS	FO	NO	DK	SE	FI
					New concentration (ng/g)						
C11H18O4	Fumaric acid, ethyl 3-methylbut-2-yl ester			0.89	89	60.0		117.0	215.0		
C11H18O4	Fumaric acid, ethyl 3-methylbut-2-yl ester			0.90			239				
C11H18O4	Fumaric acid, ethyl 3-methylbut-2-yl ester			0.91						134	97.0
C17H34O	Hexadecanal, 2-methyl-	55019-46-0		5.90	23		52			20	1,389.0
C19H40O2Si	Hexadecanoic acid, trimethylsilyl ester	55520-89-3		2.80	910	2,407.0	397	1,310.0	747.0	891	1,357.0
C9H10O2	m-Cresyl acetate	122-46-3	NS00012122	2.20						324	
C6H11N1O2	Morpholine, 4-acetyl-	1696-20-4	NS00009993	2.10					13.0		8.1
C5H9NO2	N-Formylmorpholine	4394-85-8	NS00105320	2.90	42	42.0	75	52.0	42.0	46	56.0
C18H38O2Si	n-Pentanoic acid, trimethylsilyl ester	74367-22-9		2.80	412	3,915.0	316	1,205.0	515.0		586.0
C10H21N1O1	N,N-Dimethyloctanamide	1118-92-9	NS00009475	1.80		52.0			10.0		
C10H8	Naphthalene	91-20-3	NS00008377	1.00					4.1		
C15H22	naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1s-cis)-	483-77-2	NS00095902	1.20		40.0					
C18H37NO	Octadecanamide (branched)			1.00		458.0					
C16H33N1O1	Palmitamide	629-54-9	NS00014846	0.89	135	408.0		129.0	101.0		
C9H10O2	Paroxypropione	70-70-2	NS00003309	1.20	22		183		51.0	27	5.5
C12H12O5	Phenacylidene diacetate	5062-30-6		0.89				15.0	51.0		
C12H12O5	Phenacylidene diacetate	5062-30-6		0.92						33	23.0
C14H10	Phenanthrene	85-01-8	NS00009484	1.00			37	21.0			
C8H6O2	Phenylglyoxal	1074-12-0	NS00023460	1.70	41			60.0	46.0	32	75.0
C24H38O4	Phthalic acid, di(2-propylpentyl) ester			1.20	490	3,118.0			370.0		
C24H38O4	Phthalic acid, di(6-methylhept-2-yl) ester			1.20			372				567.0
C23H36O4	Phthalic acid, hept-3-yl octyl ester			1.10				463.0		275	
C15H22O3	Salicylic acid, butyl ether, butyl ester			1.40			17	16.0	5.3		
C17H25NO4	Succinic acid, 2-(dimethylamino) ethyl 4-isopropylphenyl ester			0.84		190.0			382.0	1,374	145.0
C17H25NO4	Succinic acid, 2-(dimethylamino) ethyl 4-isopropylphenyl ester			0.80			136				
C10H14O2	tert-Butylhydroquinone	1948-33-0	NS00010294	1.90			127	192.0	166.0	118	117.0
C17H36O2Si	Tetradecanoic acid, trimethylsilyl ester	18603-17-3		3.20	5,138	5,972.0	5,837	7,850.0	1,522.0	2,842	1,922.0
C11H20	trans-Decalin, 2-methyl-	958-76-1		4.10		6,452.0					
C11H20	trans-Decalin, 2-methyl-	958-76-1		4.00			137				
C9H18Cl3O4P1	Tris(2-chloroisopropyl) phosphate (TCPP)	13674-84-5	NS00009572	3.20	62			40.0	13.0	17	26.0

3 Identify more of the compounds

3.1 Which are the sources of the compounds?

By filtering the chemicals registered with knowledge on industrial application and chemical physical characteristics, it is possible to extract more information about a compound identified to molecule level. The Swedish Chemicals Agency has produced a tool for identifying chemical compounds based on chemical registers of governmental organizations of EU, USA, China, Australian and others in addition the chemicals in commerce registry of the Swedish Chemicals Agency, see Figure 3.1. The tool merges info from these trade regulating chemicals databases with information on hazard and exposure probability drawn from the information on commercial applications in the regulatory databases as well as information on physical chemical properties and toxicological and ecotoxicological properties from the SPIN 2000 database. Where the SPIN 2000 database is a repository for data required for instance is health and safety assessments for the Classification and Labeling Directive.

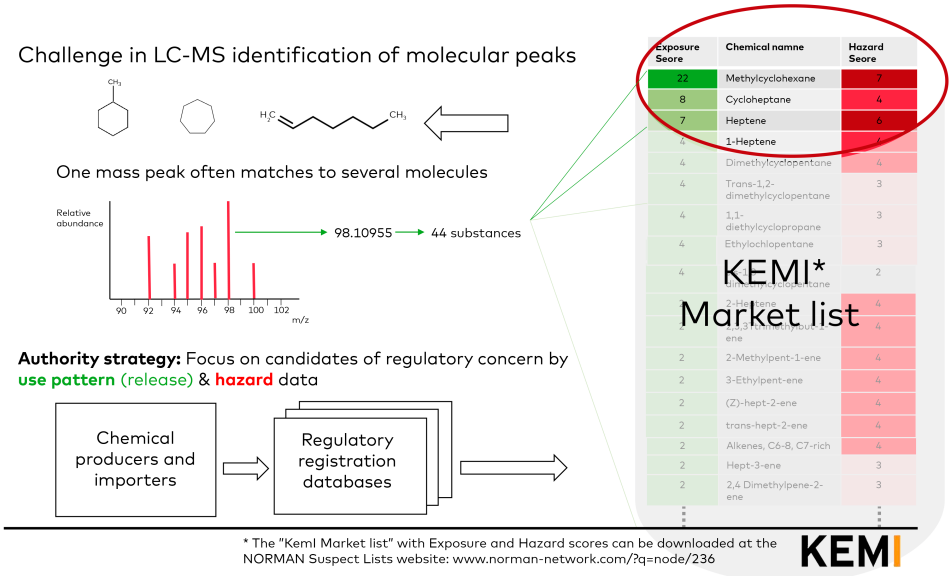

Figure 3.1 The figure describes the rationale for using a curated chemicals list for identifying a substance. (Modified from figure presented at CityLeaks seminar, Malmø 2018 by Stellan Fisher)

3.2 Suspects lists

The processes will take the form of a forward and a reversed screening approach, which may be summarized as consisting of:

1. Input MS data (empirical formulas/accurate mass) for chemical identification in the filter matrix developed by Stellan Fischer at the Swedish Environment Agency (KEMI) to select a shortlist of candidate compounds. The output of potential hits from the registry i.e. candidate chemicals may thereafter be subject to additional manual verification including for example the use of in silico tools. The latter verification process may especially be useful with the LCMS(MS) data.
2. Based on agreed parameters (i.e. select chemicals in use in relevant areas of the Nordics countries, ambient production, etc. for which the KEMI scoring system is prepared) a list of suspect compounds is produced which may subsequently be checked against digital archives (MS data). A univocal identification may require additional confirmation, as new runs on the MS with suitable standards.

3.3 Reanalyzed effluent sample data

The LC-HRMS data independent acquisition data from the effluent samples was reanalyzed using a deconvolution and a universal library search algorithm developed by Samanipour and co-workers (Samanipour et al. 2016, 2018). The scripts containing the used algorithms are available on GitHub (https://github.com/saersamani/Decon_ULSA_DIA_HRMS). The suspect list used for the reanalysis was the Norman Substance Database list (SusDat) from 2018 which had around 20000 compounds at the time, the current SusDat and other suspect lists are available at NORMAN Suspect List Exchange (https://www.norman-network.com/nds/SLE/).

The reanalysis resulted in just over 15000 unique feature identifications and of those 127 features were identified to ID Level 2 (Probable Structure, by library/diagnostic evidence) (Schymanski et al. 2015), see Table 3.1.

Table 3.1 Features identified at ID Level 2 in effluent samples using deconvoluting and library match algorithm

Name	CAS	Norman SusDat ID	GL	IS	FO	NO	DK	SE	FI
1,3-bis(2,6-dimethylphenoxy)propan-2-ol	856976-65-3	NS00008105		v	v				
1,3-diphenylguanidine	102-06-7	NS00104223	v	v	v	v	v	v	v
1011-Dihydro-1011-dihydroxycarbamazepine									v
2-{[(6-Methoxy-1H-benzimidazol-2-yl)sulfanyl]methyl}-3,5-dimethylpyridin-4(1H)-one (4-hydroxy omeprazole sulphide)	103876-98-8	NS00014620	v	v	v	v	v	v	v
2,2-Bis(hydroxymethyl)-1,3-propanediyl dioctanoate	55680-37-0	NS00033364		v	v				
3-Pyrazolidinone,1-phenyl-	92-43-3	NS00019857	v						
3,4,5-Triethoxybenzoic acid	6970-19-0	NS00036921							v
3,6,9,12,15,18,21,24,27-Nonaoxanonacosane-1,29-diol	5579-66-8	NS00001004	v	v	v	v		v	v
3,6,9,12,15,18,21,24,27,30-Decaoxadotriacontane-1,32-diol	6891-45-8	NS00001005	v	v	v	v		v	v
3,6,9,12,15,18,21,24,27,30,33,36-Dodecaoxaoctatriacontane-1,38-diol	17598-96-8	NS00001007	v	v	v				
34-Methylenedioxy-N-methylamphetamine						v	v	v	v
4-(Dipropylamino)benzenediazonium tetrafluoroborate	5059-80-3	NS00032088				v			
4-OH-Carbamazepine		NS00040768							v
5,6,7,8-Tetrahydroquinazoline-2,4-diamine	1899-40-7	NS00026209				v	v	v	v
Alfuzosin	81403-80-7	NS00000621						v	v
alpha-Ketometoprolol					v	v	v	v	v
Alverine	150-59-4	NS00010383	v	v	v	v	v	v	v
Amisulpride	71675-85-9	NS00000416		v		v	v		v
Amitriptyline	50-48-6	NS00000032		v		v	v	v	v
Arginine	7200-25-1	NS00101925	v						
Aspidospermine	466-49-9	NS00031621	v	v					
Atenolol	29122-68-7	NS00010385					v		
Azithromycin	83905-01-5	NS00000204					v	v	v
Benzoic acid, 2-(dimethylamino)-	610-16-2	NS00034525	v						
Benzoylecgonine	519-09-5	NS00000407		v		v			v
Berberine	2086-83-1	NS00009669				v			v
Bexarotene	153559-49-0	NS00000606					v		v
Bisoprolol	66722-44-9	NS00009929							v
Bupropion	34911-55-2	NS00000397							v
Caffeine	58-08-2	NS00000273	v	v	v	v	v	v	v
Carbamazepine	298-46-4	NS00000207	v	v	v	v	v	v	v
Carbamazepine-1011-epoxide			v		v	v		v	v
Carbamazepine epoxide	36507-30-9	NS00000327						v	v
Celiprolol	56980-93-9	NS00010514							v
Cetirizine	83881-51-0	NS00000386	v	v	v	v	v	v	v
Ciprofloxacin	85721-33-1	NS00008031		v		v	v		
Cis-Zeatin			v		v				
Citalopram	59729-33-8	NS00000035	v	v	v	v	v	v	v
Clarithromycin	81103-11-9	NS00000205				v	v	v	v

Name	CAS	Norman SusDat ID	GL	IS	FO	NO	DK	SE	FI
Climbazole	38083-17-9	NS00008150	v	v	v	v	v	v	v
Clomipramine	303-49-1	NS00000038							v
Clozapine	5786-21-0	NS00000413		v	v	v	v	v	v
Cocaine	50-36-2	NS00000403				v			v
Codeine	76-57-3	NS00000391	v	v	v	v	v	v	v
Colchicine	64-86-8	NS00002718				v	v		v
Cotinine	486-56-6	NS00010263	v	v	v	v	v		v
Crotamiton	483-63-6	NS00010892				v			
Cyheptamide	7199-29-3	NS00037314				v	v	v	v
DEET	134-62-3	NS00000221	v	v		v	v	v	v
Dibucaine	85-79-0	NS00010344				v			v
Diphenhydramine	58-73-1	NS00010439			v				
Disopyramide	3737-09-5	NS00003733	v	v	v	v	v	v	v
Dodecaethlene glycol (PEG-12)	25322-68-3	NS00001006	v	v	v	v			
Edifenphos	17109-49-8	NS00001472				v	v	v	v
Eprosartan	133040-01-4	NS00000388				v		v	v
Fexofenadine	83799-24-0	NS00010515	v	v	v	v	v	v	v
Finasteride	98319-26-7	NS00010893	v		v				
Flecainide	54143-55-4	NS00010512		v		v	v	v	v
Fluconazole	86386-73-4	NS00000281				v	v	v	v
Fludrocortisone	127-31-1	NS00010380	v	v		v	v		v
Furosemide	54-31-9	NS00008630			v				v
Gelsemine	509-15-9	NS00006472	v						
Hexaethylene glycol	2615-15-8	NS00001003			v	v	v	v	v
Hydroxybutorphanol								v	
Iminostilbene	256-96-2	NS00000328	v		v	v	v	v	v
Irbesartan	138402-11-6	NS00000387				v	v	v	
Ketoconazole	65277-42-1	NS00010890	v		v		v	v	
Lamotrigine	84057-84-1	NS00000354	v		v	v	v	v	v
Levamisole	14769-73-4	NS00000419				v	v	v	v
Losartan	114798-26-4	NS00008822	v	v	v	v	v		v
Meclizine	569-65-3	NS00000507	v			v	v	v	v
Methadone	76-99-3	NS00000411				v	v	v	v
Metoclopramide	364-62-5	NS00000392					v	v	v
Metoprolol	37350-58-6	NS00000197	v	v	v	v	v	v	v
Mirtazapine	85650-52-8	NS00009441	v	v	v	v	v	v	v
N-Acetylaminoantipyrine	83-15-8	NS00000226					v		v
N,N-Dimethyldodecylamine-N-oxide	1643-20-5	NS00001592		v	v				
NO-Didesmethylvenlafaxine			v	v	v	v	v	v	v
Norbuprenorphine	78715-23-8	NS00010446	v	v		v		v	v
Norclozapine	6104-71-8	NS00098561			v	v	v		v
Olopatadine	113806-05-6	NS00000615		v		v	v	v	v
Oxazepam	604-75-1	NS00007748							v

Name	CAS	Norman SusDat ID	GL	IS	FO	NO	DK	SE	FI
Oxycodone	76-42-6	NS00010443				v	v		v
Pantoprazole	102625-70-7	NS00000297	v						
PEG-12			v	v	v	v			v
PEG-15			v	v	v				
PEG-7EO			v	v	v	v	v	v	v
PEG-8EO			v	v	v	v	v	v	v
PEG-9EO			v	v	v	v	v	v	v
Phenol, 2-[(dimethylamino)methyl]-4-(1,1-dimethylethyl)-	97-43-8	NS00040516	v						
Sitagliptin	486460-32-6	NS00000425				v		v	v
Sotalol	3930-20-9	NS00000195		v	v	v	v	v	v
Sulfapyridine	144-83-2	NS00000225			v		v	v	v
Sulpiride	15676-16-1	NS00010476					v		v
Telmisartan	144701-48-4	NS00000398				v	v	v	v
Tiamulin	55297-95-5	NS00000009	v	v	v	v	v	v	v
Triamterene	396-01-0	NS00010256							v
Trimethoprim	738-70-5	NS00000211	v	v	v	v	v	v	v
Trospium	47608-32-2	NS00098770					v		v
Tyrosine	60-18-4	NS00078967	v					v	v
Valsartan	137862-53-4	NS00000341				v			v
Venlafaxine	93413-69-5	NS00000031	v	v	v	v	v	v	v
Verapamil metabolite D617	34245-14-2	NS00008205		v	v	v	v	v	v

3.4 Further curation of the detected and identified compounds list from the initial study.

The list of compounds identified to ID level 3 and above in the initial study were further curated. This was done mainly using the newest SusDat list (Network et al. 2021), where the full dataset is available for download at the NORMAN Suspect List Exchange website (https://www.norman-network.com/nds/SLE/), and the CompTox Chemicals Dashboard (Williams et al. 2017) which has an online batch search option (max 5000 at a time) (https://comptox.epa.gov/dashboard/dsstoxdb/batch_search). The lists are split into three tables, effluent (Table 6.1), biota (Table 6.2), and sediment (Table 6.3), see Appendix 6.

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Appendix

A Sample information

Table A.1 Sampling stations

Country	Location	Site	Matrix	Species
Denmark	Roskilde	Risø	Biota	Eelpout
Denmark	Aarhus	Marselisborg WWTP	Effluent	
Denmark	Roskilde	Ros 60	Sediment	
Faroe Islands	Tórshavn	VA11 and VA17	Biota	Saithe
Faroe Islands	Tórshavn	VA11 (Sersjantvíkin)	Effluent	
Faroe Islands	Tórshavn	VA 17 (Álaker)	Sediment	
Finland	Helsinki	Vanhankaupunginselkä	Biota	Perch
Finland	Helsinki	Viikinmäki	Effluent	
Finland	Helsinki	Vanhankaupunginselkä	Sediment	
Greenland	Nuuk Fiord	Kakillarnat	Biota	Cod
Greenland	Nuuk	Kakillarnat	Effluent	
Greenland	Nuuk	Kakillarnat	Sediment	
Iceland	Reykjavik	Inner Faxafloi bay	Biota	Cod
Iceland	Reykjavik	Klettagarðar WWTP	Effluent	
Iceland	Reykjavik	Inner Faxafloi bay	Sediment	
Norway	Oslo	Oslofjord	Biota	Cod
Norway	Oslo	VEAS	Effluent	
Norway	Oslo	Oslofjord	Sediment	
Sweden	Stockholm	Henriksdal WWTP	Biota	Perch
Sweden	Stockholm	Henriksdal WWTP	Effluent	
Sweden	Stockholm	Henriksdal WWTP	Sediment	

B.1 Effluent samples

Table B.1 Detected compounds in the effluent samples

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C12H20O2	(Z)-dihydro-5-(2-octenyl) furan-2(3H)-one	18679-18-0	NS00052592	2		v							
C10H22O3	1-(2-Butoxy-1-methylethoxy) propan-2-ol	29911-28-2	NS00002704	3	v	v	v			v			Misc.
C10H22O3	1-(2-Butoxy-1-methylethoxy) propan-2-ol	29911-28-2	NS00002704	2				v					Misc.
C14H9Cl2N1O1	1-(2,6-Dichlorophenyl)-2-indolinone	15362-40-0	NS00004994	3					v	v	v		PPCP
C16H11ClN3O3	1-[(2-chloro-4-nitrophenyl) azo]-2-naphthol	2814-77-9	NS00048734	2		v		v				Halogenated	
C7H4F13N1O2S1	1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-methyl-	68259-15-4	NS00011242	2				v		v			
C10H14	1,2,3,4-Tetramethylbenzene	488-23-3	NS00021173	2		v							
C10H14	1,2,3,5-Tetramethylbenzene	527-53-7	NS00009847	2		v							
C7H8O2	1,3-Benzenediol, 5-methyl-	504-15-4	NS00032059	2		v							
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	3	v	v	v		v	v	v		
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	2				v					
C18H36O3	12-hydroxystearic acid	106-14-9	NS00104291	2	v								
C20H30O2	13-ethyl-3-methoxygona-2,5(10)-dien-17Î²-ol	14507-49-4	NS00002728	2					v				
C9H7N1O1	1H-Indole-3-carboxaldehyde	487-89-8	NS00031825	2	v								
C10H9F9O2	1H,1H,2H,2H-Perfluorohexyl methacrylate	1799-84-4	NS00010989	2	v		v	v	v	v		PFAS	
C12H10O1	2'-Acetonaphthone	93-08-3	NS00004934	2							v		
C10H22O2	2-(2-Ethylhexyloxy) ethanol	1559-35-9	NS00020386	2		v							
C8H7N1S2	2-(Methylthio)benzothiazole	615-22-5	NS00007832	2		v	v		v	v	v	Industrial additive	
C16H34O3	2-[2-(Dodecyloxy) ethoxy] ethanol	3055-93-4	NS00013814	2	v								
C9H11N1O2	2-Ethoxybenzamide	938-73-8	NS00002670	2			v						
C18H26O3	2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	NS00013675	2	v								
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2		v				v			
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2		v				v			
C8H10O2	2-Phenoxyethanol	122-99-6	NS00002984	2	v	v	v		v	v	v	Germacide	Misc.
C13H10N2O3S	2-phenyl-1H-benzimidazole-5-sulphonic acid	27503-81-7	NS00106882	2						v			
C13H10N2O3S	2-phenyl-1H-benzimidazole-5-sulphonic acid	27503-81-7	NS00106882	3							v		

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C8H10O1	2-Phenylethanol	60-12-8	NS00004212	3	v	v							
C9H12O1	2-Phenylpropan-2-ol	617-94-7	NS00010783	2			v						
C10H12O2	2-Propanone, 1-(4-methoxyphenyl)-	122-84-9	NS00011990	2		v							
C14H8N2S2	2,2'-Bibenzothiazole	4271-09-4		3	v								
C12H18O1	2,4-Diisopropylphenol		NS00007254	2					v				
C16H30O2	2,5,8,11-Tetramethyldodec-6-yne-5,8-diol	68227-33-8	NS00003000	2					v				
C9H12O2	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	NS00010663	2							v	flavorant/ fragrance	Food additive
C11H13ClO	3-Buten-1-ol, 4-chloro-2-methyl-1-phenyl-			2	v					v	v	Halogenated	
C13H20O	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	NS00075791	2	v								
C7H9N1O2	3-Ethyl-4-methyl-1H-pyrrole-2,5-dione	20189-42-8	NS00010668	3	v	v	v		v	v	v		
C7H9N1O2	3-Ethyl-4-methyl-1H-pyrrole-2,5-dione	20189-42-8	NS00010668	2				v					
C12H24O3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3		2	v	v	v		v	v	v		
C12H24O3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3		3				v					
C8H8O2	3-Hydroxy-4-methylbenzaldehyde	57295-30-4	NS00076576	3		v		v					
C7H7NO2	3-Methyl-2-vinylmaleimide	21494-57-5		3		v							
C13H12	3-Methylbiphenyl	643-93-6	NS00022617	2		v							
C9H9N1	3-Methylindole	83-34-1	NS00013192	2	v		v						
C15H12Br4O2	3,3',5,5'-Tetrabromobisphenol A	79-94-7	NS00002438	2						v		Bisphenol	Flame Retardant
C15H11N1	3,3-Diphenylacrylonitrile	3531-24-6	NS00010692	3				v					
C15H11N1	3,3-Diphenylacrylonitrile	3531-24-6	NS00010692	2					v		v		
C9H18O2	3,5,5-trimethylhexanoic acid	512345	NS00105192	2					v				
C10H22O1	3,7-Dimethyl-3-octanol	78-69-3	NS00003469	2	v	v	v						PPCP
C8H10O1	4-Ethylphenol	123-07-9	NS00010739	2	v							flavorant/ fragrance	Misc.
C8H7N1O1	4-Hydroxyindole	2380-94-1	NS00013759	3	v	v							
C8H8O3	4-Hydroxyphenylacetate	3233-32-7		2	v								
C7H7N3	4-Methyl-1H-benzotriazole	29878-31-7	NS00108592	2					v				
C7H7NO5S	4-nitrotoluene-2-sulphonic acid	121-03-9	NS00104563	2	v		v						
C12H10O4S1	4,4'-Sulfonyldiphenol	80-09-1	NS00010610	2		v						Bisphenol	Misc.
C12H10O4S1	4,4'-Sulfonyldiphenol	80-09-1	NS00010610	1			v	v				Bisphenol	Misc.
C6H5F9O	4:2 FTOH	2043-47-2	NS00108564	3							v	PFAS	
C11H20O2	5-Heptyldihydro-2(3H)-furanone	104-67-6	NS00008440	2	v							Fragrance	Misc.
C6H7N5S1	6-Methylthioguanine	1198-47-6	NS00008363	2						v			
C6H6N4O2	7-Methylxanthine	552-62-5	NS00005508	2						v			
C14H11N	9-methylacridine	611-64-3	NS00042821	2	v			v	v	v	v	PAC	

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C14H26O2	9-Tetradecenoic acid, (9Z)-	544-64-9	NS00020426	2	v								
C12H12O	a-methylnaphthalene-2-methanol	7228-47-9	NS00044941	2							v		
C18H28N2O4	Acebutolol	37517-30-9	NS00006043	2				v		v	v	Drug	PPCP
C13H13N3O3S1	Acetamide, N-[4-[(2-pyridinylamino) sulfonyl]phenyl]-	19077-98-6	NS00008156	2						v			
C13H13N3O3S1	Acetamide, N-[4-[(2-pyridinylamino) sulfonyl]phenyl]-	19077-98-6	NS00008156	3							v		
C8H9N1O2	Acetaminophen	103-90-2	NS00000231	2	v	v	v						PPCP
C20H23N1	Amitriptyline	50-48-6	NS00000032	2		v	v	v	v	v	v	Drug	PPCP
C20H25Cl1N2O5	Amlodipine	88150-42-9	NS00000043	2	v	v	v		v	v	v	Drug	PPCP
C38H52N6O7	Atazanavir	198904-31-3	NS00000470	2	v			v	v	v	v	Drug	PPCP
C14H22N2O3	Atenolol	29122-68-7	NS00010385	2	v	v	v	v	v	v	v	Drug	PPCP
C38H72N2O12	Azithromycin	83905-01-5	NS00000204	2		v	v	v	v	v	v	Drug	PPCP
C8H12N2O3	Barbital	57-44-3	NS00003391	2				v					
C17H28	BENZENE, (1-BUTYLHEPTYL)-	4537-15-9	NS00095862	2	v								
C18H30	BENZENE, (1-PENTYLHEPTYL)-	2719-62-2	NS00008712	2	v								
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		2	v	v				v	v		
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		3				v					
C15H13N1	Benzenepropanenitrile, . beta.-phenyl-	61310-06-3	NS00010691	2		v		v	v	v	v		
C9H11N1O2	Benzocaine	94-09-7	NS00001814	2	v					v		Drug	PPCP
C22H36O2	Benzoic acid, pentadecyl ester		NS00076547	3	v	v	v		v	v			
C22H36O2	Benzoic acid, pentadecyl ester		NS00076547	2				v					
C20H32O2	Benzoic acid, tridecyl ester		NS00076546	3	v	v	v	v	v	v	v		
C13H10O1	Benzophenone	119-61-9	NS00010632	2	v	v	v	v	v	v	v		PPCP
C7H5N1O1S1	Benzothiazolone	934-34-9	NS00008199	3	v					v			PPCP
C16H19N1O4	Benzoylecgonine	519-09-5	NS00000407	2		v		v	v	v	v		
C9H10O2	Benzyl acetate	140-11-4	NS00002107	2		v						Fragrance	PPCP
C18H14F4N2O4S1	Bicalutamide	90357-06-5	NS00000400	2					v	v			
C15H24	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9		2	v								
C24H38O4	Bis(2-ethylhexyl) terephthalate	6422-86-2	NS00007552	3	v								Misc.
C13H12O2	Bis(4-hydroxyphenyl) methane	620-92-8	NS00009451	1		v		v		v		Bisphenol	Plastic manufacturing
C13H12O2	Bis(4-hydroxyphenyl) methane	620-92-8	NS00009451	2							v	Bisphenol	Plastic manufacturing
C18H31N1O4	Bisoprolol	66722-44-9	NS00009929	2				v	v	v	v	Drug	PPCP
C12H11N3O3S1	C.I. Food Yellow 6	104-23-4	NS00006633	2						v		Colorant	PPCP
C12H11N3O3S1	C.I. Food Yellow 6	104-23-4	NS00006633	3							v	Colorant	PPCP
C8H10N4O2	Caffeine	58-08-2	NS00000273	3	v	v	v		v	v	v		PPCP
C8H10N4O2	Caffeine	58-08-2	NS00000273	2	v	v	v	v	v	v	v		PPCP

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C11H10N4O4	Carbadox	6804-07-5	NS00011822	2						v			
C15H12N2O1	Carbamazepine	298-46-4	NS00000207	2	v	v	v	v	v	v	v	Drug	PPCP
C15H14N2O2	Carbamazepine, 10-hydroxy			2	v	v	v	v	v	v	v		
C15H14N2O3	Carbamazepine, 10, 11-dihydroxy			2	v	v	v	v	v	v	v		
C20H33N3O4	Celiprolol	56980-93-9	NS00010514	2				v	v	v	v	Drug	PPCP
C21H25Cl1N2O3	Cetirizine	83881-51-0	NS00000386	2	v	v	v	v	v	v	v	Drug	PPCP
C15H11Cl1O3	Chlorflurenol-methyl	2536-31-4	NS00002592	2		v		v					
C17H18F1N3O3	Ciprofloxacin	85721-33-1	NS00008031	2	v	v	v	v	v	v	v	Drug	PPCP
C20H21F1N2O1	Citalopram	59729-33-8	NS00000035	2	v	v	v	v	v	v	v	Drug	PPCP
C38H69N1O13	Clarithromycin	81103-11-9	NS00000205	2		v	v	v	v	v	v	Drug	PPCP
C18H19Cl1N4	Clozapine	5786-21-0	NS00000413	2	v	v	v	v	v	v	v	Drug	PPCP
C17H21N1O4	Cocaine	50-36-2	NS00000403	2		v		v	v	v	v	Drug - Illicit	PPCP
C18H21N1O3	Codeine	76-57-3	NS00000391	2		v	v	v	v	v	v	Drug	PPCP
C10H12N2O1	Cotinine	486-56-6	NS00010263	2	v	v	v	v	v	v	v	Tobacco	PPCP
C9H6O2	Coumarin	91-64-5	NS00002381	2	v	v	v						PPCP
C18H10	Cyclopenta[cd]pyrene	27208-37-3	NS00005566	2					v				
C18H26O1	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	1222-05-5	NS00008760	2	v		v	v	v	v	v		PPCP
C6H12O6	D-Glucose	50-99-7	NS00007629	2		v							
C7H9N1O2	Deferiprone	30652-11-0	NS00005705	2			v			v			
C19H19F1N2O1	desmethylcitalopram	62498-67-3	NS00006900	2	v				v	v	v	Drug	PPCP
C22H26N2O4S1	Diltiazem	56209-45-1	NS00000473	2		v	v	v	v	v	v	Drug	PPCP
C8H14O4	Dimethyl adipate	627-93-0	NS00004584	3	v	v				v	v		
C8H14O4	Dimethyl adipate	627-93-0	NS00004584	2				v					
C24H40N8O4	Dipyridamol			2		v	v	v			v		
C22H43NO	docos-13-enamide, Amides, C22 (unsaturated)			2						v			
C12H24O2	Dodecanoic acid	143-07-7	NS00008441	2	v								
C16H30O2	dodecyl methacrylate	142-90-5	NS00104758	2		v			v				
C13H10N2O3S1	Ensulizole	27503-81-7	NS00010386	2			v	v	v	v			PPCP
C13H10N2O3S1	Ensulizole	27503-81-7	NS00010386	3							v		PPCP
C23H24N2O4S1	Eprosartan	133040-01-4	NS00000388	2				v		v	v	Drug	PPCP
C8H8O2	Ethanone, 2-hydroxy-1-phenyl-	582-24-1	NS00022418	2	v	v	v	v	v	v	v		
C17H21N1O3	Etodolac	41340-25-4	NS00010209	2					v				
C32H39N1O4	Fexofenadine	83799-24-0	NS00010515	2	v	v	v	v	v	v	v	Drug	PPCP
C17H20F6N2O3	Flecainide	54143-55-4	NS00010512	2		v		v	v	v	v	Drug	PPCP
C13H12F2N6O1	Fluconazole	86386-73-4	NS00000281	2					v				
C17H34O	Hexadecanal, 2-methyl-	55019-46-0		2	v								
C17H34O	Hexadecanal, 2-methyl-	55019-46-0		2	v								
C16H32O2	Hexadecanoic acid	57-10-3	NS00008548	2			v	v				Saturated fatty acid	Misc.
C19H40O2Si	Hexadecanoic acid, trimethylsilyl ester	55520-89-3		2	v	v	v	v	v	v	v		

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C7H8Cl1N3O4S2	Hydrochlorothiazide	58-93-5	NS00000343	2		v			v	v		Halogenated	
C7H8Cl1N3O4S2	Hydrochlorothiazide	58-93-5	NS00000343	3							v	Halogenated	
C18H21N1O3	Hydrocodone	125-29-1	NS00009201	2		v	v	v	v	v	v		
C20H40O2	icosanoic acid	506-30-9	NS00107202	2		v				v			
C8H7N1	Indole	120-72-9	NS00010849	2	v								
C9H7N1O1	Indole-4-carboxaldehyde	1047-86-6	NS00015304	2	v	v	v	v	v	v			
C10H12N4O5	Inosine	58-63-9	NS00010210	3							v		
C25H28N6O1	Irbesartan	138402-11-6	NS00000387	2		v		v	v		v	Drug	PPCP
C8H5N1O2	Isatin	91-56-5	NS00005535	3	v								
C17H34O2	isopentyl laurate	6309-51-9	NS00107436	2		v	v	v					
C15H30O2	isopropyl laurate	10233-13-3	NS00104226	2				v					
C17H34O2	Isopropyl tetradecanoate	110-27-0	NS00006471	2		v	v	v					Misc.
C26H28Cl2N4O4	Ketoconazole	65277-42-1	NS00010890	2	v	v	v	v	v	v	v		
C9H11N1O3	L-threo-3-Phenylserine	69-96-5	NS00002730	2			v						
C11H12N2O2	l-Tryptophan	73-22-3	NS00003513	2			v					amino acid	PPCP
C9H7Cl2N5	Lamotrigine	84057-84-1	NS00000354	2	v	v	v	v	v	v	v		
C24H48O2	Lauryl laurate	13945-76-1	NS00009876	2						v			
C22H23Cl1N6O1	Losartan	114798-26-4	NS00008822	2	v	v	v	v	v	v	v		
C7H8O1	m-Cresol	108-39-4	NS00010658	2	v					v		flavorant/ fragrance	Misc.
C7H8O1	m-Cresol	108-39-4	NS00010658	3				v				flavorant/ fragrance	Misc.
C20H23N1	Maprotiline	10262-69-8	NS00009793	2		v	v	v	v	v	v		
C11H15N1O2	MDMA	42542-10-9	NS00010441	2		v		v	v	v	v		
C10H20O1	Menthol (DL-menthol)	89-78-1	NS00001027	2	v	v	v						PPCP
C20H30O2	metenolone	153-00-4	NS00077347	2					v				
C21H27N1O1	Methadone	76-99-3	NS00000411	2				v	v	v	v		
C20H28O2	Methandrostenolone	72-63-9	NS00010330	2					v				
C8H9N1O2	Methyl 2-aminobenzoate	134-20-3	NS00002018	2	v								
C9H18O2	Methyl 2-ethylhexanoate	816-19-3	NS00001346	2					v				
C5H8O3	methyl acetoacetate	105-45-3	NS00104278	2				v		v			
C15H30O2	methyl myristate	124-10-7	NS00104609	2				v					
C9H18O2	methyl octanoate	111-11-5	NS00104427	2					v				
C17H34O2	methyl palmitate	112-39-0	NS00104480	2		v	v						
C14H22Cl1N3O2	Metoclopramide	364-62-5	NS00000392	2		v	v	v	v	v	v		
C15H25N1O3	Metoprolol	37350-58-6	NS00000197	2	v	v	v	v	v	v	v		
C17H19N3	Mirtazapine	85650-52-8	NS00009441	2	v	v	v	v	v	v	v		
C10H15N1O2S1	N-Butylbenzenesulfonamide	3622-84-2	NS00007746	2	v			v	v				
C17H17Cl1N4	N-Desmethylclozapine	6104-71-8	NS00010419	2		v	v	v	v	v	v	Drug	PPCP
C5H9NO2	N-Formylmorpholine	4394-85-8	NS00105320	2		v				v	v		
C18H38O2Si	n-Pentanoic acid, trimethylsilyl ester	74367-22-9		2	v	v				v	v		
C14H31N1	N,N-Dimethyldodecan-1-amine	112-18-5	NS00006542	3			v						
C10H8	Naphthalene	91-20-3	NS00008377	2		v							
C9H18O2	Neononanoic acid	59354-78-8	NS00004316	2					v				

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C10H14N2	Nicotine	54-11-5	NS00010445	2	v	v	v	v	v	v	v	Drug	PPCP
C9H18O2	Nonanoic acid	112-05-0	NS00009752	2					v				
C16H25N1O2	O-Desmethyl Venlafaxine	93413-62-8	NS00000330	2	v	v	v	v	v	v	v	Drug	PPCP
C16H32O2	octyl octanoate	2306-88-9	NS00106773	2			v	v					
C17H20N4S1	Olanzapine	132539-06-1	NS00000036	3							v		
C17H19N3O4S1	Omeprazole sulfone	88546-55-8	NS00003072	3							v		
C29H44O12	Ouabain	630-60-4	NS00003260	2		v							
C15H11Cl1N2O2	Oxazepam	604-75-1	NS00007748	2		v	v	v	v	v	v		PPCP
C7H8O1	p-Cresol	106-44-5	NS00008242	2	v								Misc.
C7H6O2	p-Hydroxybenzaldehyde	123-08-0	NS00014566	2	v	v	v	v	v	v		Flavorant/ Colorant	PPCP
C7H6O2	p-Hydroxybenzaldehyde	123-08-0	NS00014566	3							v	Flavorant/ Colorant	PPCP
C9H19NO4	panthenol, DL-form	16485-10-2	NS00106616	2			v			v			PPCP
C15H28O2	Pentadecan-15-olide	106-02-5	NS00007638	2				v					Misc.
C12H12O5	Phenacylidene diacetate	5062-30-6		2		v							
C24H26O2	Phenol, 4,4'-[1,3-phenylenebis(1-methylethylidene)]bis-	13595-25-0	NS00006040	2		v		v				Bisphenol	
C24H26O2	Phenol, 4,4'-[1,3-phenylenebis(1-methylethylidene)]bis-	13595-25-0	NS00006040	1			v		v	v		Bisphenol	
C7H5N1O1	Phenyl isocyanate	103-71-9	NS00010655	2				v					
C8H6O2	Phenylglyoxal	1074-12-0	NS00023460	2	v		v		v	v	v		
C8H6O2	Phenylglyoxal	1074-12-0	NS00023460	3				v					
C6H2F13O3P1	Phosphonic acid, (tridecafluorohexyl)-		NS00011279	2						v		PFAS	
C6H2F13O3P1	Phosphonic acid, (tridecafluorohexyl)-		NS00011279	3							v	PFAS	
C23H36O4	Phthalic acid, hept-3-yl octyl ester			2	v								
C8H5N1O2	Phthalimide	85-41-6	NS00010682	2			v			v			
C12H26O4S.K	Potassium dodecyl sulphate	4706-78-9	NS00081255	2					v	v			
C12H26O4S.K	Potassium dodecyl sulphate	4706-78-9	NS00081255	3							v		
C16H21N1O2	Propranolol	525-66-6	NS00000196	2	v	v	v	v	v	v	v	Drug	PPCP
C6H7NS	Pyridine, 2-(methylthio)-	18438-38-5		2				v	v	v	v		
C21H25N3O2S1	Quetiapine	111974-69-7	NS00010395	2	v	v	v	v	v	v	v	Drug	PPCP
C20H24N2O2	Quinine	130-95-0	NS00002397	2	v	v	v	v	v	v	v	Drug	PPCP
C14H9Cl1F3N1O3	rac 8-Hydroxy Efavirenz	205754-32-1	NS00009526	2						v			
C6H6O2	Resorcinol	108-46-3	NS00007013	2		v							
C15H22O3	Salicylic acid, butyl ether, butyl ester			2	v								
C16H15F6N5O1	Sitagliptin	486460-32-6	NS00000425	2		v		v	v	v	v	Drug	PPCP
C12H20N2O3S1	Sotalol	3930-20-9	NS00000195	2		v	v	v	v	v	v	Drug	PPCP
C18H36O2	stearic acid	57-11-4	NS00105495	2		v				v			
C17H25NO4	Succinic acid, 2-(dimethylamino) ethyl 4-isopropylphenyl ester			2	v								

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C11H11N3O2S1	Sulfapyridine	144-83-2	NS00000225	2	v	v	v	v	v	v	v	Drug	PPCP
C14H12O6S	sulisobenzone	4065-45-6	NS00107115	2						v			
C14H12O6S1	Sulisobenzone	4065-45-6	NS00009581	2				v	v	v			PPCP
C14H12O6S1	Sulisobenzone	4065-45-6	NS00009581	3							v		PPCP
C15H23N3O4S1	Sulpiride	15676-16-1	NS00010476	2				v	v	v	v	Drug	PPCP
C14H21N3O2S1	Sumatriptan	103628-46-2	NS00009397	2	v	v	v	v	v	v	v	Drug	PPCP
C33H30N4O2	Telmisartan	144701-48-4	NS00000398	2		v		v	v	v	v	Drug	PPCP
C14H28O2	Tetradecanoic acid	544-63-8	NS00010444	2				v					
C17H36O2Si	Tetradecanoic acid, trimethylsilyl ester	18603-17-3		2	v	v	v			v	v		
C14H30O4S1	Tetradecyl sulfate	4754-44-3	NS00005015	2					v			Drug	PPCP
C16H25N1O2	Tramadol	27203-92-5	NS00000338	2	v	v	v	v	v	v	v	Drug	PPCP
C12H22O2	trans-4-tert-butylcyclohexyl acetate	1900-69-2	NS00081890	2	v		v						
C9H14O6	Triacetin	102-76-1	NS00010706	2		v				v	v		Misc.
C9H14O6	Triacetin	102-76-1	NS00010706	3				v					Misc.
C10H14O	tricyclo[5.2.1.0(2,6)]dec-3-en-10-ol	39852-87-4	NS00096343	3	v	v							
C2H1F3O2	Trifluoroacetic acid	76-05-1	NS00008877	2						v			
C14H18N4O3	Trimethoprim	738-70-5	NS00000211	2	v	v	v	v	v	v	v	Drug	PPCP
C10H14O2Si	Trimethylsilyl benzoate	2078-12-8	NS00045989	2		v							
C21H44O2Si	Trimethylsilyl stearate	18748-91-9	NS00048143	2		v		v		v	v		
C13H28O4	Tripropylene glycol butyl ether	55934-93-5	NS00001901	2	v								
C18H39O7P1	Tris(2-butoxyethyl) phosphate	78-51-3	NS00010389	2				v			v		
C9H18Cl3O4P1	Tris(2-chloroisopropyl) phosphate (TCPP)	13674-84-5	NS00009572	2	v				v	v	v	Halogenated flame retardant	Misc.
C9H6O3	Umbelliferone	93-35-6	NS00001324	2		v						Natural product	PPCP
C18H28O2	Undecyl benzoate	6316-30-9	NS00096101	3	v	v	v	v	v	v	v		PPCP
C24H29N5O3	Valsartan	137862-53-4	NS00000341	2		v		v	v	v	v	Drug	PPCP
C24H29N5O3	Valsartan	137862-53-4	NS00000341	3							v	Drug	PPCP
C17H27N1O2	Venlafaxine	93413-69-5	NS00000031	2	v	v	v	v	v	v	v	Drug	PPCP

B.2 Biota samples

Table B.2 Detected compounds in the biota samples

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C8H18N2O4S1	(4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid	7365-45-9	NS00004939	3							v		
C8H12O	(E,E)-3,5-Octadien-2-one	30086-02-3		2	v	v	v	v		v	v		
C6H6N2O2	(Pyrimidin-2-yl)acetic acid	66621-73-6		3					v	v	v		
C9H17N1O4	(S)-2-((tert)-butoxycarbonyl)amino)butanoic acid	34306-42-8	NS00004773	3					v				
C10H22O3	1-(2-Butoxy-1-methylethoxy) propan-2-ol	29911-28-2	NS00002704	3					v				Misc.
C9H10O3	1-(2,4-Dihydroxy-3-methylphenyl) ethanone	10139-84-1		2		v		v	v	v	v		
C17H24O1	1-(6-tert-Butyl-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl) ethanone	13171-00-1	NS00001394	3		v							Musk comp
C16H11ClN3O3	1-[(2-chloro-4-nitrophenyl) azo]-2-naphthol	2814-77-9	NS00048734	3							v	Halogenated	
C12H8Br2O	1-Bromo-2-(4-bromophenoxy) benzene	147217-71-8	NS00077051	2	v	v	v	v				PBDE	
C14H14	1,1'-Biphenyl, 2,3'-dimethyl-	611-43-8		2					v	v	v		
C14H14	1,1'-Biphenyl, 2,4'-dimethyl-	611-61-0		2					v	v	v		
C7H5NS	1,2-Benzisothiazole	272-16-2		2	v		v	v					
C13H16	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6	NS00022016	2	v					v	v		
C13H18	1,2,3,4-Tetrahydro-1,6,8-trimethylnaphthalene	30316-36-0		2	v								
C7H8O2	1,3-Benzenediol, 5-methyl-	504-15-4	NS00032059	2					v	v			
C8H9NO4	1,4-dimethoxy-2-nitrobenzene	89-39-4	NS00105984	3				v					
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	3	v		v						
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	2				v					
C23H40O3	11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	71041-49-1		2	v	v		v		v	v	Furan fatty acid	
C21H36O3	11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	86879-46-1		2	v	v		v		v	v	Furan fatty acid	
C9H8O1	1H-Inden-1-one, 2,3-dihydro-	83-33-0	NS00038249	2					v	v			
C8H7N1S2	2-(Methylthio)benzothiazole	615-22-5	NS00007832	2				v	v	v		Industrial additive	

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C12H15N5O5	2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl]methoxy]ethyl acetate	75128-73-3	NS00107617	3	v						v		
C16H34O3	2-[2-(Dodecyloxy)ethoxy]ethanol	3055-93-4	NS00013814	2	v								
C10H10ClN3O2	2-chloro-6,7-dimethoxyquinazolin-4-amine	23680-84-4	NS00106784	3			v					Halogenated	
C12H22	2-Ethyldecahydronaphthalene, (Z,E)-	66660-41-1		2		v	v						
C9H8O3	2-Hydroxy-5-methylisophthalaldehyde	7310-95-4	NS00037473	2						v			
C7H5N1S2	2-Mercaptobenzothiazole	149-30-4	NS00000568	2				v				Industrial additive	
C9H10O3	2-methoxy-6-methylbenzoic acid	6161-65-5	NS00107392	3							v		
C9H16O2	2-methylcyclohexyl acetate	5726-19-2	NS00009395	3	v								
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2					v				
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2					v				
C8H10O2	2-Phenoxyethanol	122-99-6	NS00002984	2							v	Germicide	Misc.
C9H8O	2-Phenylpropenal	4432-63-7	NS00076572	2	v	v		v	v				
C11H16O2	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	17092-92-1		2	v	v			v				
C14H8N2S2	2,2'-Bibenzothiazole	4271-09-4		3					v				
C12H24N2O3	2,2'-dimorpholinyldiethyl ether	6425-39-4	NS00107461	3							v	Catalyst	Construction
C12H3Cl7	2,2',3,3',4,4',5-Heptachloro-1,1'-biphenyl (PCB 170)	35065-30-6	NS00114249	2	v	v	v	v	v	v	v	PCB	
C12H2Cl8	2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB194)	35694-08-7	NS00114174	2	v	v	v	v	v	v	v	PCB	
C12HCl9	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB 206)	40186-72-9	NS00114147	2	v	v	v	v	v	v	v	PCB	
C12H4Cl6	2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)	35065-28-2	NS00005294	2	v	v	v	v	v	v	v	PCB	
C12H3Cl7	2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	NS00001212	2	v	v	v	v	v	v	v	PCB	
C12H5Cl5	2,2',3,4,6-Pentachlorobiphenyl	55215-17-3		2				v		v	v	PCB	
C12H4Br6O1	2,2',4,4',5,5'-Hexabromodiphenyl ether	68631-49-2	NS00008955	2	v	v	v	v	v	v	v	PBDE	
C12H4Cl6	2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)	35065-27-1	NS00005442	2	v	v	v	v	v	v	v	PCB	
C12H6Cl4	2,2',5,5'-Tetrachlorobiphenyl (PCB 52)	35693-99-3	NS00001956	3	v	v	v	v	v	v	v	PCB	
C15H28	2,2,4,4,7,7-Hexamethyloctahydro-1H-indene	54832-83-6		3		v	v						
C12H6Br4O1	2,3',4,4'-Tetrabromodiphenyl ether	189084-61-5	NS00001012	2	v	v	v	v	v	v	v	PBDE	
C12H5Cl5	2,3',4,4',5-Pentachlorobiphenyl (PCB 118)	31508-00-6	NS00001962	2	v	v		v	v	v	v	PCB	

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C12H5Cl5	2,3',4,4',5-Pentachlorobiphenyl (PCB 118)	31508-00-6	NS00001962	2	v	v		v	v	v	v	PCB	
C12H4Cl6	2,3',4,4',5,5'-Hexachlorobiphenyl (PCB 167)	52663-72-6	NS00099486	2	v	v	v	v	v	v	v	PCB	
C12H22	2,3-Dimethyldecahydronaphthalene	1008-80-6		3		v	v						
C12H5Cl5	2,3,3',4,4'-Pentachlorobiphenyl (PCB 105)	32598-14-4	NS00114177	2		v		v	v	v	v	PCB	
C12H4Cl6	2,3,3',4,4',5-Hexachlorobiphenyl (PCB 156)	38380-08-4	NS00003535	2	v	v	v	v	v	v	v	PCB	
C12H3Cl7	2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9	NS00074014	2	v	v	v	v	v	v	v	PCB	
C12H4Cl6	2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8		2		v		v		v	v	Halogenated	
C6H4Br2O1	2,4-Dibromophenol	615-58-7	NS00001617	2	v	v	v	v	v	v	v	Halogenated	Flame Retardant
C7H5Br3O1	2,4,6-Tribromoanisole	607-99-8	NS00003721	2	v	v	v	v	v	v	v	Natural product	
C6H3Br3O1	2,4,6-Tribromophenol	118-79-6	NS00004395	2	v	v	v	v	v	v	v	Halogenated	Flame Retardant
C16H20	2,6-Diisopropylnaphthalene	24157-81-1	NS00010761	2		v					v		Pesticide
C9H12O2	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	NS00010663	2	v				v	v	v	flavorant/ fragrance	Food additive
C7H5F9O2	3-(Perfluorobutyl)propanoic acid	80705-13-1	NS00011089	2						v		PFAS	
C13H20O	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	NS00075791	2	v	v		v					
C12H24O3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3		2	v	v	v	v	v	v	v		
C7H7NO2	3-Methyl-2-vinylmaleimide	21494-57-5		3					v				
C12H6Br4O	3,3',4,4'-Tetrabromodiphenyl ether	93703-48-1	NS00074031	2	v	v	v	v	v	v	v	PBDE	
C15H12Br4O2	3,3',5,5'-Tetrabromobisphenol A	79-94-7	NS00002438	2	v	v	v	v	v	v	v	Bisphenol	Flame Retardant
C8H16O	3,4-dimethylcyclohexan-1-ol	5715-23-1	NS00046141	2	v	v	v	v		v			
C16H24O2	3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	NS00108535	3			v						
C8H10O1	4-Ethylphenol	123-07-9	NS00010739	2				v				flavorant/ fragrance	Misc.
C7H6O3	4-Hydroxybenzoic acid	99-96-7	NS00005418	3			v						
C25H18O2	4,4'-(9H-Fluorene-9,9-diyl) diphenol	26088-14-2	NS00001837	3				v					
C14H14	4,4'-Dimethylbiphenyl	613-33-2	NS00034646	2					v	v	v		
C12H10O4S1	4,4'-Sulfonyldiphenol	80-09-1	NS00010610	1	v		v					Bisphenol	Misc.
C5H9N1O2	4,4-dimethyl-1,2-oxazolidin-3-one	81778-07-6	NS00005019	3							v		

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C15H12N2O3	5-(4-hydroxyphenyl)-5-phenylhydantoin	2784-27-2	NS00007796	3		v							PPCP
C6H8O3	5-acetyldihydrofuran-2(3H)-one	29393-32-6	NS00049070	2					v	v	v		
C6H13N1O2	6-Aminocaproic acid	60-32-2	NS00014764	3	v	v		v		v		Drug	PPCP
C22H30O3	6,7-DIHYDROCANRENONE	976-70-5	NS00008961	3			v						
C17H16Cl1N3O2	8-Hydroxyamoxapine	61443-78-5	NS00010101	3			v						
C12H8O4	8-Methoxypsoralen	298-81-7	NS00004875	3							v		
C10H5F17O3S1	8:2 Fluorotelomer sulfonic acid	39108-34-4	NS00011092	2							v	PFAS	
C14H26O2	9-Tetradecenoic acid, (9Z)-	544-64-9	NS00020426	2	v	v		v		v	v		
C20H32O2	Abiet-8(14)-en-18-oic acid (NSC18746)	34434-80-5	NS00001533	3			v			v			
C9H16O3	Acetic acid, 2-(cyclohexyloxy)-, methyl ester	65593-73-9	NS00004583	3		v							
C8H16N2O3	acetyllysine	692-04-6	NS00008574	3				v					
C5H4N4O1	Allopurinol	315-30-0	NS00000618	3							v	Drug	PPCP
C10H12N4O5	Allopurinol riboside	16220-07-8	NS00004733	3					v		v		
C33H33N3O1	alpha,alpha-bis[4-(Dimethylamino)phenyl]-4-(phenylamino)-1-naphthalenemethanol	6786-83-0	NS00011486	3				v					
C17H28	BENZENE, (1-BUTYLHEPTYL)-	4537-15-9	NS00095862	2		v	v						
C18H30	BENZENE, (1-PENTYLHEPTYL)-	2719-62-2	NS00008712	2		v	v						
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		2				v		v	v		
C32H37N1O4	Benzeneacetic acid, 4-[4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-Î±,Î±-dimethyl-	76811-98-8	NS00004579	3					v				
C15H13N1	Benzenepropanenitrile, .beta.-phenyl-	61310-06-3	NS00010691	2				v					
C7H6O2	Benzoic acid	65-85-0	NS00008785	2	v	v	v	v	v	v	v		Misc.
C11H14O3	Benzoic acid, 4-hydroxy-2-methyl-5-(1-methylethyl)- (9CI)	584-44-1		3	v		v						
C20H32O2	Benzoic acid, tridecyl ester		NS00076546	3							v		
C13H10O1	Benzophenone	119-61-9	NS00010632	2		v							PPCP
C7H5N1S1	Benzothiazole	95-16-9	NS00000291	2			v	v		v	v	PAC	
C7H5N1O1S1	Benzothiazolone	934-34-9	NS00008199	3	v				v	v			PPCP
C9H10O2	Benzyl acetate	140-11-4	NS00002107	2				v	v		v	Fragrance	PPCP
C13H20O1	beta-Ionone	79-77-6	NS00001727	2	v								Misc.
C15H24	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9		2	v	v	v						

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C18H20O2	Bisphenol Z	843-55-0	NS00014633	1	v	v	v					Bisphenol	
C4H6O4	Butanedioic acid	110-15-6	NS00002272	3							v		
C8H14O3	butyric anhydride	106-31-0	NS00104298	3	v								
C8H10N4O2	Caffeine	58-08-2	NS00000273	3			v						PPCP
C15H12N2O2	Carbamazepine epoxide	36507-30-9	NS00000327	3						v			PPCP
C5H9N1O4S1	Carbocysteine	2387-59-9	NS00006061	3					v				
C15H14O6	Cianidanol	154-23-4	NS00004541	3		v						Natural product	
C18H26O1	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	1222-05-5	NS00008760	2		v	v	v		v			PPCP
C9H13N3O5	Cytarabine	147-94-4	NS00005949	3				v					
C4H9NO3	D,L-4-amino-3-hydroxybutyric acid	352-21-6	NS00079381	3						v	v		
C12Cl10	Decachlorobiphenyl	2051-24-3	NS00026668	2	v	v	v	v	v	v	v	PCB	
C11H20	Decahydro-2-methylnaphthalene	2958-76-1	NS00096217	2		v	v						
C11H18O4	diethyl 1,2-cyclopentanedicarboxylate	90474-13-8	NS00004507	3	v								
C14H29NO7Si	Diethyl N-[3-(trimethoxysilyl)propyl]-L-aspartate	192389-48-3		3		v							
C15H21N1O1S1	Dimepiperate	61432-55-1	NS00008312	3					v				
C13H17N1O4	Dimethachlor OXA	1086384-49-7	NS00000332	3	v								
C19H22N2O3S1	Dimethoxanate	477-93-0	NS00006617	3				v					
C5H8O4	dimethyl malonate	108-59-8	NS00104361	3			v						
C20H32O5	Dinoprostone	363-24-6	NS00009026	3			v						
C17H26O4	Embelin	550-24-3	NS00010319	3				v			v		
C26H45N1O7S1	Ethanesulfonic acid, 2-[[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-	81-24-3	NS00002884	3				v			v	Bile	PPCP
C8H8O2	Ethanone, 2-hydroxy-1-phenyl-	582-24-1	NS00022418	2						v			
C20H28O3	Etienic acid	302-97-6	NS00011524	3	v								
C11H18O4	Fumaric acid, ethyl 3-methylbut-2-yl ester			2	v	v	v	v		v	v		
C10H13N5O5	Guanosine	118-00-3	NS00009027	3							v		
C17H34O	Hexadecanal, 2-methyl-	55019-46-0		2	v		v			v	v		
C17H34O	Hexadecanal, 2-methyl-	55019-46-0		2	v		v			v	v		
C16H32O2	Hexadecanoic acid	57-10-3	NS00008548	3							v	Saturated fatty acid	Misc.
C19H38O2	Hexadecanoic acid, 1-methylethyl ester	142-91-6	NS00009869	3							v		
C19H40O2Si	Hexadecanoic acid, trimethylsilyl ester	55520-89-3		2	v	v	v	v		v	v		

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C6H9N3O2	Histidine	4998-57-6	NS00005578	3							v		
C9H7N1O1	Indole-4-carboxaldehyde	1047-86-6	NS00015304	3	v	v	v		v	v	v		
C10H12N4O5	Inosine	58-63-9	NS00010210	3				v	v				
C11H14O3	Isobutylparaben	4247-02-3	NS00007256	3	v								
C11H12N2O2	l-Tryptophan	73-22-3	NS00003513	3							v	amino acid	PPCP
C9H10O2	m-Cresyl acetate	122-46-3	NS00012122	2						v			
C10H14O3	Mephenesin	59-47-2	NS00001081	3	v								
C14H16Cl1N3O1	Metazachlor	67129-08-2	NS00000249	3	v							Halogenated	
C6H9N1O2	methyl 2-cyano-2-methylpropanoate	72291-30-6	NS00009466	3							v		
C5H9NO2	methyl 3-aminocrotonate	14205-39-1	NS00100158	3							v		
C19H38O2	methyl isostearate	68517-10-2	NS00107532	3							v		
C19H38O2	Methyl stearate	112-61-8	NS00001076	3							v		
C6H11N1O2	Morpholine, 4-acetyl-	1696-20-4	NS00009993	3					v		v		
C5H9NO2	N-(2-hydroxyethyl) prop-2-enamide	7646-67-5	NS00105781	3							v		
C5H9NO2	N-(hydroxymethyl)methacrylamide	923-02-4	NS00107796	3							v		
C11H20N2O5	N-[N-[(1,1-dimethylethoxy) carbonyl]-L-alanyl]-L-alanine	27317-69-7	NS00004174	3							v		
C5H9NO2	N-Formylmorpholine	4394-85-8	NS00105320	2	v	v	v	v	v	v	v		
C18H38O2Si	n-Pentanoic acid, trimethylsilyl ester	74367-22-9		2	v	v	v	v	v		v		
C10H16N2O4	N,N'-ethylenebis[N-acetylacetamide]	10543-57-4	NS00104277	3							v		
C22H43NO3	N,N-bis(2-hydroxyethyl)oleamide	93-83-4	NS00079032	3				v					
C10H21N1O1	N,N-Dimethyloctanamide	1118-92-9	NS00009475	2		v			v				
C10H8	Naphthalene	91-20-3	NS00008377	2					v				
C15H22	naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1s-cis)-	483-77-2	NS00095902	2		v							
	Natural product, Br3Cl3, probably monoterpene			5		v	v	v				Natural product	
C9H20O4S1	nonyl hydrogen sulfate	26856-96-2	NS00005697	3			v						
C18H37NO	Octadecanamide (branched)			3		v							
C18H26O3	Octinoxate	5466-77-3	NS00004841	3	v								
C14H24N2O4	Oseltamivir acid	187227-45-8	NS00000302	3		v						Drug	PPCP
C5H4N4O2	Oxypurinol	2465-59-0	NS00006655	3							v		PPCP
C7H8O1	p-Cresol	106-44-5	NS00008242	3						v	v		Misc.
C7H6O2	p-Hydroxybenzaldehyde	123-08-0	NS00014566	2		v						Flavorant/ Colorant	PPCP
C7H6O2	p-Hydroxybenzaldehyde	123-08-0	NS00014566	3			v	v	v	v	v	Flavorant/ Colorant	PPCP
C16H33N1O1	Palmitamide	629-54-9	NS00014846	2	v	v		v	v			Primary fatty acid	

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C9H10O2	Paroxypropione	70-70-2	NS00003309	2	v		v		v	v	v		PPCP
C12H4Cl6	PCB-157	69782-90-7	NS00099774	2	v	v	v	v	v	v	v	PCB	
C12H2Cl8	PCB-195	52663-78-2		3	v	v	v	v	v	v	v	PCB	
C12H5Br5O1	Pentabromodiphenyl Ether	60348-60-9	NS00004728	2	v	v	v	v	v	v	v	PBDE	
C23H15N3O1	Perampanel	380917-97-5	NS00004827	3						v			
C12F23O2	Perfluorododecanoate	171978-95-3		2						v	v	PFAS	
C6H1F13O3S1	Perfluorohexanesulfonic acid	355-46-4	NS00010279	2						v	v	PFAS	
C8H1F17O3S1	Perfluorooctanesulfonic acid	1763-23-1	NS00010280	3							v	PFAS	
	PFNS	474511-07-4		2						v	v	PFAS	
C12H12O5	Phenacylidene diacetate	5062-30-6		2				v	v	v	v		
C14H10	Phenanthrene	85-01-8	NS00009484	2			v	v				PAH and alkylated derivatives	Misc.
C24H26O2	Phenol, 4,4'-[1,3-phenylenebis(1-methylethylidene)]bis-	13595-25-0	NS00006040	1	v		v	v				Bisphenol	
C8H6O2	Phenylglyoxal	1074-12-0	NS00023460	2	v			v	v	v	v		
C24H38O4	Phthalic acid, di(2-propylpentyl) ester			2	v	v							
C24H38O4	Phthalic acid, di(6-methylhept-2-yl) ester			2			v				v		
C23H36O4	Phthalic acid, hept-3-yl octyl ester			2				v		v			
C23H32N2O4	Pinoxaden	243973-20-8	NS00000321	3						v		Phenylpyrazolin	Herbicide
C15H10F6O2	Potassium 4,4'-(hexafluoroisopropylidene)diphenolate	25088-69-1	NS00011437	1	v	v		v				Bisphenol	
C31H48O2S2	Probucol	23288-49-5	NS00003652	3							v	Drug	PPCP
C11H22O3	Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester, (2S)-	186817-80-1	NS00104915	3				v					
C8H11N1O3	Pyridoxine	65-23-6	NS00004187	3							v	Vitamin	PPCP
C9H7NO	quinolin-8-ol	148-24-3	NS00106573		v								
C22H32O2	retinyl acetate	127-47-9	NS00077313	3							v		
C15H22O3	Salicylic acid, butyl ether, butyl ester			2			v	v	v				
C25H37N1O4	Salmeterol	89365-50-4	NS00010340	3						v			
C18H36O2	stearic acid	57-11-4	NS00105495	3							v		
C17H25NO4	Succinic acid, 2-(dimethylamino) ethyl 4-isopropylphenyl ester			2		v	v			v	v		
C10H14O2	tert-Butylhydroquinone	1948-33-0	NS00010294	3			v	v				synthetic aromatic organic compound	Misc.

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C10H14O2	tert-Butylhydroquinone	1948-33-0	NS00010294	2					v	v	v	synthetic aromatic organic compound	Misc.
C17H36O2Si	Tetradecanoic acid, trimethylsilyl ester	18603-17-3		2	v	v	v	v		v	v		
C9H14O3	Tetrahydrofurfuryl methacrylate	2455-24-5	NS00006075	3							v		
C10H10O	Tetralinone	529-34-0	NS00108646	3		v						Drug intermediate	PPCP
C11H20	trans-Decalin, 2-methyl-	958-76-1		2		v	v						
C8H21NOSi2	trimethylsilyl N-trimethylsilylacetamidate	10416-59-8	NS00106215	3							v		
C9H18Cl3O4P1	Tris(2-chloroisopropyl) phosphate (TCPP)	13674-84-5	NS00009572	2	v			v	v	v	v	Halogenated flame retardant	Misc.
C9H17N1O3S1	Tropine-3-mesylate	35130-97-3	NS00001123	3						v			

B.3 Sediment samples

Table B.3 Detected compounds in the sediment samples

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C13H10O1	[1,1'-Biphenyl]-4-carboxaldehyde	3218-36-8	NS00008757	2			v	v	v	v			
C16H11ClN3O3	1-[(2-chloro-4-nitrophenyl) azo]-2-naphthol	2814-77-9	NS00048734	2			v					Halogenated	
C4H10O3S1	1-Butanesulfonic acid	2386-47-2	NS00002697	2			v						
C11H14O4	1-Methyl-1,3-cyclohexadiene-5,6-diol diacetate			3					v	v	v		
C18H22	1-Methyl-7-(propan-2-yl)-1,2,3,4-tetrahydrophenanthrene	6566-19-4		3			v		v	v	v		
C15H12	1-Methyl phenanthrene	832-69-9	NS00007467	2			v		v	v		PAH and alkylated derivatives	
C18H11F19O2	1-Phenoxy(3-(perfluoro-7-methyloctyl) propan-2-ol)	94159-92-9	NS00010924	2							v		
C12H6Cl4	1,1'-Biphenyl, 2,2',5,5'-tetrachloro- (PCB-52) (isomer)			3	v				v	v	v	PCB	
C9H6F12O1	1,1,2,2,3,3,4,4,5,5,6,6-Dodecafluoro-7-(vinyloxy)heptane	78971-81-0	NS00011205	2							v		
C13H16	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6	NS00022016	2					v	v			
C16H16	1,2-Diphenylcyclobutane, cis-	7694-30-6	NS00095944	2			v	v	v	v	v		
C13H18	1,2,3,4-Tetrahydro-1,6,8-trimethylnaphthalene	30316-36-0		2					v	v			
C10H14	1,2,3,4-Tetramethylbenzene	488-23-3	NS00021173	2			v		v	v	v		
C10H14	1,2,3,5-Tetramethylbenzene	527-53-7	NS00009847	2			v		v	v			
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	2	v								
C10H16	1,5-Cyclooctadiene, 1,5-dimethyl-	3760-14-3	NS00030225	3			v		v	v	v		
C16H11N	11H-Benzo[a]carbazole (isomer)			3			v		v	v			
C16H11N	11H-Benzo[a]carbazole (isomer)-Birgitta1			3			v	v			v		
C16H11N	11H-Benzo[a]carbazole (isomer)-Birgitta2			3					v	v	v		
C21H14	13H-dibenzo[a,h]fluorene	239-85-0	NS00041490	3			v	v	v	v	v		
C9H8O1	1H-Inden-1-one, 2,3-dihydro-	83-33-0	NS00038249	2					v	v			
C9H7N1O1	1H-Indole-3-carboxaldehyde	487-89-8	NS00031825	2				v	v	v	v		
C8H7N1S2	2-(Methylthio)benzothiazole	615-22-5	NS00007832	2				v			v	Industrial additive	
C8H5Br2N	2-Bromo-6-(3-bromo-prop-1-ynyl)-pyridine			3			v	v				Halogenated	
C12H22	2-Ethyldecahydronaphthalene, (Z, E)-	66660-41-1		2					v	v			

Molecular Formula	Name	CAS	Norman SusDat ID	ID Level	GL	IS	FO	NO	DK	SE	FI	Comp. Info	Potential Source
C18H18	2-Isopropyl-10-methylphenanthrene	66552-97-4		3			v	v	v	v	v		
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2		v	v	v	v	v	v		
C11H10	2-Methylnaphthalene	91-57-6	NS00002503	2		v	v	v	v	v	v		
C8H10O2	2-Phenoxyethanol	122-99-6	NS00002984	2			v	v	v	v		Germicide	Misc.
C9H14O4	2-Propenoic acid, 2-[2-(ethenyloxy)ethoxy] ethyl ester	86273-46-3	NS00002987	2			v						
C20H14	2,2'-binaphthalene	612-78-2	NS00042025	3				v	v	v	v		
C12H5Cl5	2,2',3,4,6-Pentachlorobiphenyl	55215-17-3		2			v					PCB	
C12H6Cl4	2,2',5,5'-Tetrachlorobiphenyl (PCB 52)	35693-99-3	NS00001956	3	v	v	v		v	v	v	PCB	
C15H28	2,2,4,4,7,7-Hexamethyloctahydro-1H-indene	54832-83-6		3			v		v	v	v		
C17H12	2,3-Benzofluorene	243-17-4	NS00004617	2			v	v	v	v	v		
C6H5Cl2N1	2,3-Dichloroaniline	608-27-5	NS00008299	2					v	v		Halogenated	
C12H22	2,3-Dimethyldecahydronaphthalene	1008-80-6		3					v	v			
C12H5Cl5	2,3,3',4,4'-Pentachlorobiphenyl (PCB 105)	32598-14-4	NS00114177	2			v		v	v		PCB	
C17H16	2,3,5-Trimethylphenanthrene	3674-73-5	NS00095846	2			v	v	v	v	v	PAH and alkylated derivatives	
C13H14	2,3,6-Trimethylnaphthalene	829-26-5	NS00038227	2			v	v	v	v	v		
C10H12O1	2,4,6-Trimethylbenzaldehyde	487-68-3	NS00001558	3					v	v	v		
C16H20	2,6-Diisopropylnaphthalene	24157-81-1	NS00010761	2	v		v		v	v			Pesticide
C9H12O2	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	NS00010663	2		v	v	v	v	v	v	flavorant/ fragrance	Food additive
C13H8F21O5P1	3-(Perfluorodecyl)-2-hydroxypropyl dihydrogen phosphate	94158-70-0	NS00010951	2					v	v			
C13H20O	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	NS00075791	2					v	v	v		
C13H16O5	3-Ethoxy-4-ethoxycarbonylphenylacetic acid	99469-99-5	NS00006678	2					v	v	v		
C7H9N1O2	3-Ethyl-4-methyl-1H-pyrrole-2,5-dione	20189-42-8	NS00010668	3	v		v	v	v	v	v		
C7H9N1O2	3-Ethyl-4-methyl-1H-pyrrole-2,5-dione	20189-42-8	NS00010668	2		v							
C12H24O3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3		2	v	v	v		v	v	v		
C7H6O2	3-hydroxybenzaldehyde	100-83-4	NS00104202	2			v						
C7H7NO2	3-Methyl-2-vinylmaleimide	21494-57-5		3	v		v	v	v	v	v		
C13H12	3-Methylbiphenyl	643-93-6	NS00022617	2			v		v	v	v		
C9H9N1	3-Methylindole	83-34-1	NS00013192	2					v	v			
C15H12	3-Methylphenanthrene	832-71-3	NS00038244	2			v		v	v	v	PAH and alkylated derivatives	
C8H16O	3,4-dimethylcyclohexan-1-ol	5715-23-1	NS00046141	2					v	v			
C6H4Cl3N1	3,4,5-Trichloroaniline	634-91-3	NS00008472	2					v	v		Halogenated	

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C16H14	3,6-Dimethylphenanthrene	1576-67-6	NS00025130	2			v	v	v	v	v	PAH and alkylated derivatives	
C14H12S	3,7-Dimethyldibenzothiophene	1136-85-2		2			v		v	v	v		
C8H8O3	4-Hydroxy-3-methoxybenzaldehyde	121-33-5	NS00009754	2					v	v	v	Flavorant	PPCP
C8H7N1O1	4-Hydroxyindole	2380-94-1	NS00013759	3		v			v	v			
C15H12	4-Methylphenanthrene	832-64-4	NS00002091	2			v	v	v	v	v	PAH and alkylated derivatives	
C20H16	4,12-Dimethyltetraphene	35187-19-0		3			v		v	v	v		
C14H14	4,4'-Dimethylbiphenyl	613-33-2	NS00034646	2			v		v	v	v		
C12H10O4S1	4,4'-Sulfonyldiphenol	80-09-1	NS00010610	1		v						Bisphenol	Misc.
C30H48O	4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one			3					v	v	v		
C6H3F9O1	4:2 Fluorotelomer aldehyde	135984-67-7	NS00011080	2				v				PFAS	
C15H8O1	4H-Cyclopenta(def)phenanthren-4-one	5737-13-3	NS00014588	2			v	v	v	v	v		
C11H20O2	5-Heptyldihydro-2(3H)-furanone	104-67-6	NS00008440	2					v	v		Fragrance	Misc.
C11H16O2	5,6,7,7a-tetrahydro-4,4,7a-trimethylbenzofuran-2(4H)-one	15356-74-8	NS00051943	2			v	v	v	v	v	flavorant/ fragrance	Food additive
C21H36	5a-pregnane	641-85-0	NS00042173	3			v		v	v	v		
C16H11N1	5H-Benzo(b)carbazole	243-28-7	NS00027618	2					v	v	v		
C15H10	6H-Cyclobuta[jk]phenanthrene	83469-43-6		2			v	v	v	v	v		
C17H12	7H-Benzo[c]fluorene (isomer)			3			v	v	v	v	v		
C17H12	7H-Benzo[c]fluorene (isomer)-Birgitta			3			v	v	v	v	v		
C17H12	7H-Benzo[c]fluorene (isomer)-Birgitta2			3			v				v		
C17H12	7H-Benzo[c]fluorene (isomer)-Birgitta3			3							v		
C17H12	7H-Benzo[de]anthracene	199-94-0		3			v		v	v	v		
C19H14	8,9-Dihydro-7H-cyclopenta[a]pyrene	82979-72-4		3			v	v	v	v	v		
C15H12	8,9-Dihydrocyclopenta[def]phenanthrene	27410-55-5		3			v	v	v	v	v		
C10H5F17O3S1	8:2 Fluorotelomer sulfonic acid	39108-34-4	NS00011092	2							v	PFAS	
C21H14	8H-Indeno[2,1-b] phenanthrene	241-28-1		3			v		v	v	v		
C19H12	9H-Cyclopenta[a]pyrene	50861-05-7		2			v	v	v	v	v		
C13H10O1	9H-Xanthene	92-83-1	NS00019926	2			v	v	v	v	v	Dye precursor	
C16H12	Acephenanthrylene, 4,5-dihydro-	6232-48-0		2			v	v	v	v	v		
C16H10S	Anthra(1,2-b) thiophene	227-86-1		3				v	v	v	v		
C14H10	Anthracene	120-12-7	NS00010699	2		v	v	v	v	v	v	PAH - Dye precursor	Misc.
C14H8O2	Anthraquinone	84-65-1	NS00010810	2			v	v	v	v	v	Mineral	Misc.
C18H12	Benz(a)anthracene	56-55-3	NS00010721	2		v	v	v	v	v	v		
C17H11N1	Benz[c]acridine	225-51-4	NS00014411	3					v	v			

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C17H10O1	Benz[de]anthracen-7-one	82-05-3	NS00003051	2				v	v	v	v		
C17H28	BENZENE, (1-BUTYLHEPTYL)-	4537-15-9	NS00095862	2			v		v	v	v		
C18H30	BENZENE, (1-PENTYLHEPTYL)-	2719-62-2	NS00008712	2		v	v		v	v	v		
C14H14O	Benzene, 1-methyl-2-(phenylmethoxy)-	19578-70-2		2		v	v		v	v	v		
C20H12	Benzo(a)pyrene	50-32-8	NS00006321	2			v	v	v	v	v		
C21H14	Benzo(a)pyrene, 10-methyl-	63104-32-5		3			v		v	v	v		
C20H12	Benzo(b)fluoranthene	205-99-2	NS00006596	2			v	v	v	v	v	PAC	
C17H12S	Benzo(b)naphtho(2,1-d) thiophene, 2-methyl-			3			v		v	v	v		
C16H10O1	Benzo(b)naphtho(2,3-d) furan	243-42-5	NS00027627	3			v		v	v	v		
C20H12	Benzo(e)pyrene	192-97-2	NS00002471	2			v	v	v	v	v		
C16H10O	Benzo(k l)xanthene	200-23-7	NS00041302	3				v	v	v	v		
C20H12	Benzo(k)fluoranthene	207-08-9	NS00003847	2					v	v			
C16H10O	Benzo[b]naphtho[1,2-d] furan	205-39-0		3			v	v	v	v	v		
C16H10S	Benzo[b]naphtho[1,2-d] thiophene	205-43-6		2			v	v	v	v	v		
C16H10S1	Benzo[b]naphtho[2,1-d] thiophene	239-35-0	NS00027512	2				v	v	v	v		
C18H14S	benzo[b]naphtho[2,3-d] thiophene, 6,8-dimethyl-	24964-16-7	NS00095900	3			v		v	v	v		
C18H12	Benzo[c]phenanthrene	195-19-7	NS00041480	2			v	v	v	v	v		
C18H10	Benzo[ghi]fluoranthene	203-12-3	NS00041486	2			v		v	v	v		
C20H12	Benzo[j]fluoranthene	205-82-3	NS00041304	2			v		v	v	v		
C7H6O2	Benzoic acid	65-85-0	NS00008785	2			v						Misc.
C22H36O2	Benzoic acid, pentadecyl ester		NS00076547	3	v	v	v		v	v	v		
C20H32O2	Benzoic acid, tridecyl ester		NS00076546	3	v	v	v				v		
C13H10O1	Benzophenone	119-61-9	NS00010632	2	v	v	v	v	v	v	v		PPCP
C7H5N1S1	Benzothiazole	95-16-9	NS00000291	2	v	v	v		v	v	v	PAC	
C13H20O1	beta-Ionone	79-77-6	NS00001727	2					v	v			Misc.
C15H24	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9		2		v	v		v	v			
C24H38O4	Bis(2-ethylhexyl) terephthalate	6422-86-2	NS00007552	3			v		v	v			Misc.
C13H12O2	Bis(4-hydroxyphenyl) methane	620-92-8	NS00009451	2				v				Bisphenol	Plastic manufacturing
C12H1F26O2P1	Bis(tridecafluorohexyl)phosphinic acid		NS00011284	2							v	PFAS	
C18H20O2	Bisphenol Z	843-55-0	NS00014633	1		v			v	v	v	Bisphenol	
C18H26O1	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	1222-05-5	NS00008760	2			v		v	v			PPCP
C11H20	Decahydro-2-methylnaphthalene	2958-76-1	NS00096217	2			v				v		
C12H8O1	Dibenzofuran	132-64-9	NS00010742	2			v	v	v	v	v	Heterocyclic organic compound	
C13H16O	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-	55591-10-1		3				v	v	v	v		

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C8H8O2	Ethanone, 2-hydroxy-1-phenyl-	582-24-1	NS00022418	2			v		v	v	v		
C16H10	Fluoranthene	206-44-0	NS00010700	2		v	v	v	v	v	v	PAC	
C13H10	Fluorene	86-73-7	NS00010698	2			v	v	v	v	v	PAH	
C11H18O4	Fumaric acid, ethyl 3-methylbut-2-yl ester			2			v		v	v	v		
C19H40O2Si	Hexadecanoic acid, trimethylsilyl ester	55520-89-3		2	v	v	v		v	v	v		
C30H50	Hop-22(29)-ene	1615-91-4		3			v		v	v	v		
C22H12	Indeno(1,2,3-cd) fluoranthene	193-43-1	NS00073880	2			v		v	v	v		
C22H12	Indeno(1,2,3-cd) pyrene	193-39-5	NS00008394	2			v		v	v	v		
C8H7N1	Indole	120-72-9	NS00010849	2		v			v	v			
C9H7N1O1	Indole-4-carboxaldehyde	1047-86-6	NS00015304	2	v		v	v	v	v	v		
C11H14O3	Isobutylparaben	4247-02-3	NS00007256	2					v	v			
C20H30O2	Isopimaric acid	5835-26-7	NS00022421	2		v	v	v			v		
C30H48O	Lup-20(29)-en-3-one	1617-70-5		3					v	v	v		
C7H4Cl1N1O1	m-Chlorophenyl isocyanate	2909-38-8	NS00007754	3					v	v		Halogenated	
C5H10O4S	mercaptoacetic acid, monoester with propane-1,2,3-triol	30618-84-9	NS00106955	2			v						
C9H10O2	Methyl phenylacetate	101-41-7	NS00001353	2					v	v	v	flavorant/ fragrance	Misc.
C6H11N1O2	Morpholine, 4-acetyl-	1696-20-4	NS00009993	3							v		
C5H9NO2	N-Formylmorpholine	4394-85-8	NS00105320	2		v					v		
C10H8	Naphthalene	91-20-3	NS00008377	2			v		v	v	v		
C15H22	naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1s-cis)-	483-77-2	NS00095902	2			v		v	v	v		
C12H12	Naphthalene, dimethyl-Birgitta1			3			v	v	v	v	v		
C12H12	Naphthalene, dimethyl-Birgitta2			3			v	v	v	v	v		
C18H10O1	Naphtho(2,1,8,7-klmn) xanthene	191-37-7	NS00026242	3			v	v	v	v	v		
C7H8O1	p-Cresol	106-44-5	NS00008242	2					v	v			Misc.
C7H6O2	p-Hydroxybenzaldehyde	123-08-0	NS00014566	2	v	v	v	v	v	v	v	Flavorant/ Colorant	PPCP
C12H1F23O2	Perfluorododecanoic acid	307-55-1	NS00009617	2							v	PFAS	
C6H1F13O3S1	Perfluorohexanesulfonic acid	355-46-4	NS00010279	2							v	PFAS	
C8H2F17N1O2S1	Perfluorooctanesulfonamide	754-91-6	NS00010967	2				v				PFAS	
C20H12	Perylene	198-55-0	NS00007842	2			v	v	v	v	v		Misc.
C6HF11O2	PFHxA	307-24-4	NS00104040	2			v	v	v	v	v	PFAS	
	PFNS	474511-07-4		2							v	PFAS	
C12H12O5	Phenacylidene diacetate	5062-30-6		2			v				v		
C13H8O	Phenalen-1-one	548-39-0	NS00043912	2			v	v	v	v	v		
C14H10	Phenanthrene	85-01-8	NS00009484	2		v	v	v	v	v	v	PAH and alkylated derivatives	Misc.

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C16H14	Phenanthrene, 4,5-dimethyl- (8CI) (9CI)	3674-69-9	NS00095887	2			v	v	v	v	v	PAH and alkylated derivatives	
C15H12	Phenanthrene, methyl-			3				v				PAH and alkylated derivatives	
C6H5Br1O1	Phenol, 3-bromo-	591-20-8	NS00034092	2		v	v					Halogenated	
C24H26O2	Phenol, 4,4'-[1,3-phenylenebis(1-methylethylidene)] bis-	13595-25-0	NS00006040	1		v			v	v	v	Bisphenol	
C24H38O4	Phthalic acid, di(2-propylpentyl) ester			2				v					
C23H36O4	Phthalic acid, hept-3-yl octyl ester			2	v	v	v		v	v	v		
C22H34O4	Phthalic acid, nonyl 2-pentyl ester			2					v	v	v		
C15H10F6O2	Potassium 4,4'-(hexafluoroisopropylidene)diphenolate	25088-69-1	NS00011437	1							v	Bisphenol	
C16H10	Pyrene	129-00-0	NS00010701	2		v	v	v	v	v	v	PAH	Misc.
C15H22O3	Salicylic acid, butyl ether, butyl ester			2			v		v	v	v		
C15H14N4O2S1	Sulfaphenazole	526-08-9	NS00006369	2			v						
C12H22O2	trans-4-tert-butylcyclohexyl acetate	1900-69-2	NS00081890	2					v	v			
C11H20	trans-Decalin, 2-methyl-	958-76-1		2					v	v			
C9H14O6	Triacetin	102-76-1	NS00010706	2			v		v	v	v		Misc.
C21H44O2Si	Trimethylsilyl stearate	18748-91-9	NS00048143	2			v						
C18H12	Triphenylene	217-59-4	NS00026961	2		v	v	v	v	v	v	PAH	
C9H18Cl3O4P1	Tris(2-chloroisopropyl) phosphate (TCPP)	13674-84-5	NS00009572	2	v	v	v		v	v	v	Halogenated flame retardant	Misc.
C18H28O2	Undecyl benzoate	6316-30-9	NS00096101	3	v	v	v		v	v	v		PPCP

About this publication

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