Greenpeace Research Laboratories Analytical Results 2017-02

Organic contaminants and metals arising in wastewater samples from an industrial site in Slovakia

May 2017

Introduction

16 samples of wastewater were received from Greenpeace CEE (Slovakia) for analysis at the Greenpeace Research Laboratories on 24 February 2017. According to documentation supplied, all samples were collected between 21st and 22nd of February, 2017, from the industrial site Fortischem, a. s. (District of Nováky town, see Box 1).

Details of the samples received are provided in Table 1a, together with GPS coordinates for the sample collection location in Table 1b. All samples were collected from a treated wastewater discharge drain from a waste water treatment plant (WWTP) at the site as described below, and at approximately 3-hour intervals, from 14:00 on 21st February to 14:10 on 22nd February 2017.

At each sampling time, two water samples were collected:

- a single 500ml sample (SK17001a to SK17008a) for quantitative analysis for dissolved metals and for qualitative analysis for the presence of solvent-extractable semi-volatile organic compounds (sVOCs) and
- a single 50ml sample (SK17001b to SK17008b) for qualitative analysis for the presence of volatile organic compounds (VOCs), in addition to a quantitative analysis for a range of VOCs classified as common environmental contaminants.

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Box 1: Description of Fortischem, a. s. industrial site

There are several plants operating at the Fortischem, a. s. industrial site, which between them manufacture a range of chemicals, including the following:

Manufacture of inorganic chemicals, organic chemicals, polymers and PVC processing products, such as:

1. chloroparaffins
2. dichlorethane, and vinyl chloride from dichlorethane
3. NaOH, hydrogen, chlorine, NaClO, drying and liquefaction of chlorine, manufacture of HCl
4. calcium carbide and C_2H_2
5. propylene oxide, polyether polyols and amines
6. PVC and initiators
7. PVAL/PVAC
8. acetylenic alcohols
9. Ethylene Chlorhydrin and its processing into 'Novamal'
10. vinyl chloride from acetylene

At this industrial site, there is a wastewater treatment plant (WWTP) which treats both wastewater from industrial processes and domestic sewage from the facilities. It was effluent from this WWTP that was sampled on 8 occasions in this study, at the point at which the treated effluent is finally discharged to the environment.

Sample code	Date & time	Analyses conducted
SK17001a	**14:00, 21.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17001b		VOCs (qualitative and quantitative)
SK17002a	**17:10, 21.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17002b		VOCs (qualitative and quantitative)
SK17003a	**21:10, 21.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17003b		VOCs (qualitative and quantitative)
SK17004a	**00:10, 22.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17004b		VOCs (qualitative and quantitative)
SK17005a	**03:10, 22.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17005b		VOCs (qualitative and quantitative)
SK17006a	**06:10, 22.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17006b		VOCs (qualitative and quantitative)
SK17007a	**10:30, 22.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17007b		VOCs (qualitative and quantitative)
SK17008a	**14:10, 22.02.2017**	metals (quantitative) & sVOCs (qualitative)
SK17008b		VOCs (qualitative and quantitative)

Table 1a: details of samples received and analysed at the Greenpeace Research Laboratories

Sample code	N			E		
	degree (º)	minutes (')	seconds ('')	degree (º)	minutes (')	seconds ('')
SK17001-8	48	41	51.48	018	31	18.30

Table 1b: GPS coordinates of sample collection location

Materials and methods

Dissolved concentrations of metals and metalloids were determined for all samples by ICP mass spectrometry (MS) following acid digestion and using appropriate laboratory reference samples. Hexavalent chromium concentrations in filtered samples were determined colourimetrically using a diphenylcarbazide method. The samples visually contained only minor traces of suspended matter and, therefore, concentrations of metals in whole (unfiltered samples) were not separately determined.

sVOCs were isolated from each sample using solid phase extraction (SPE), eluting with ethyl acetate, pentane and toluene. Extracted compounds were subsequently identified as far as possible using gas chromatography/mass spectrometry (GC/MS). Volatile organic chemicals (VOCs) were identified and quantified in samples as received (with no pre-treatment) using GC/MS with HeadSpace sample introduction technique. Quantification of a selection of the VOCs detected was carried out using internal standards calibration. More detailed descriptions of the sample preparation and analytical procedures are presented in Appendix 1.

Results and Discussion

The results for the samples are outlined in the following sections. The dissolved concentrations of metals and metalloids in filtered samples are reported in Table 2. In addition, the organic chemicals identified in individual samples are summarised in Tables 3 (for sVOCs) and 4 (for VOCs). The results for quantitative VOCs analysis are presented in Table 5. The temporal trends of major contaminants over the 24-hour sampling period are presented in Figure 1 (for metals/metalloids), Figure 2 (for major sVOCs) and Figure 3 (for major quantified VOCs) respectively. A full list of organic chemicals identified in each sample is provided in Appendix 2.

In some cases, concentrations of metals or metalloids were below limits of detection for the analytical methods employed in this study. These are shown in the results tables as '<xx' where xx is the method detection limit for the individual metal or metalloid.

3.1 Metals

Over the sampling period, the wastewater was commonly alkaline in nature, with pH ranging from 8.4 to 11.3, but with one very notable exception; sample SK17004, collected just after midnight on 22nd February 2017, was highly acidic, with a pH of only 1.4, perhaps indicative of a periodic discharge from a specific industrial process on the site or a marked change in the treatment processes applied to the wastewater around that time (see Table 2).

In general, concentrations of the metals/metalloids <u>other than mercury</u> that were quantified in the samples showed little sign of elevation in concentrations above typical background concentrations for uncontaminated surface freshwaters (see e.g. Salomons & Forstner 1984, ATSDR 2005a/b, Comber *et al.* 2008). Concentrations of barium in all filtered samples (in the range from 103 µg/L to 1290 µg/L, respectively) fell in the wide range reported for raw surface waters and public drinking water supplies (≤5 to 15,000 µg/l), but were higher than reported average (mean) concentrations for such waters, which are generally in the order of 10–60 µg/l (ATSDR 2007).

Concentrations of several metals, including aluminium (Al, 308 µg/l), chromium (Cr, 4.3 µg/l), iron (Fe, 975 µg/l), lead (Pb, 2.8 µg/l) and zinc (Zn, 65 µg/l) were higher in that acidic sample (SK17004) than in the other 7 samples, as may be expected from the higher solubility of these metals in acidic compared to alkaline conditions. As for the pH data, the data on metals concentrations for this sample suggest markedly different inputs to the wastewater, or of treatment processes applied to the wastewater, during this period. Nonetheless, concentrations of aluminium and iron similar to, or above, those in SK17004 can be found naturally in surface waters under more acidic conditions (ATSDR 2008).

By far the greatest concern, however, were the very high concentrations of the toxic metal mercury (Hg) found in all of the samples, ranging from 14 µg/l to 487 µg/l, and with an average concentration of 236 µg/l across the 8 samples.

All samples exceed background levels reported for freshwaters without known sources of mercury contamination (Gilmour & Henry 1991, Hope & Rubin 2005) of total mercury by more than 1000 times. In the case of the sample SK17008, the concentration of mercury was almost 100 000 times above this level for uncontaminated freshwaters (0.005 µg/l).

	Concentration, µg/l							
Sample code	SK17001	SK17002	SK17003	SK17004	SK17005	SK17006	SK17007	SK17008
Aluminium (Al)	24	<10	44	308	<10	22	27	24
Antimony (Sb)	0.4	0.6	0.7	<0.1	0.8	0.9	1.0	1.2
Arsenic (As)	8.8	2.0	2.0	8.8	2.2	2.5	2.0	5.7
Barium (Ba)	103	351	575	1290	921	951	1080	1220
Beryllium (Be)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
Cadmium (Cd)	<0.02	<0.02	<0.02	0.03	<0.02	<0.02	<0.02	<0.02
Chromium (Cr)	0.4	0.3	0.3	4.3	0.4	0.4	0.4	1.1
Chromium (VI)	<50	<50	<50	<50	<50	<50	<50	<50
Cobalt (Co)	0.12	0.07	0.08	0.30	0.11	0.10	0.09	0.28
Copper (Cu)	1.6	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	0.9
Iron (Fe)	171	<10	19	975	23	13	<10	91
Lead (Pb)	0.5	<0.5	<0.5	2.8	<0.5	<0.5	<0.5	<0.5
Manganese (Mn)	114	<0.1	<0.1	205	<0.1	<0.1	<0.1	<0.1
Mercury (Hg)	14	190	272	16	310	139	462	487
Nickel (Ni)	1.2	0.6	0.6	4.7	1.0	0.6	0.7	1.7
Selenium (Se)	0.2	0.5	0.8	0.3	0.8	0.8	0.8	1.0
Vanadium (V)	<1	<1	<1	<1	<1	<1	<1	<1
Zinc (Zn)	23	<0.5	<0.5	65	<0.5	1.2	3.9	1.1
pH	8.46	9.42	9.69	1.40	9.25	9.42	10.85	11.33

Table 2: Concentrations of metals and metalloids (µg/l) in filtered wastewater samples, and their pH values.

The concentrations of the other metals/metalloids quantified in the samples indicated that wastewaters were not notably contaminated with these metals, with little sign of elevation in concentrations above typical background concentrations for uncontaminated surface freshwaters (see e.g. Salomons & Forstner 1984, ATSDR 2005a/b, Comber *et al.* 2008).

3.2 Organic contaminants

3.2.1 Semi-volatile organic compounds

As all samples were collected from the same pipe at different time, the composition of organic compounds detected in them showed some similarity (see Table 3). All samples contained a range of chlorinated and non-chlorinated organic contaminants, clearly indicating that the treatment techniques used for these wastewaters before they have been discharged are not able to break down or otherwise remove such contaminants effectively. Due to the complexity of the patterns of chemical contamination of these samples, from the relatively high number of compounds isolated in the samples (from 62 to 102), it was possible to identify to a high degree of reliability only between 13% and 28%.

Among the contaminants detected in the wastewater at least at one of the sampling times were:

- Diethyl phthalate (DEP), well known as a plasticizer in a variety of products including for cellulose ester plastic films and sheets. It is also used as an ingredient in a range of cosmetic formulations and, in particular, in nail polish as a solvent for nitrocellulose and cellulose acetate, in perfumes as a fixative and solvent, and in toilet preparations as an alcohol denaturant (ATSDR 1995).
- Propane, 2,2'-oxybis[1-chloro- has a variety of applications including as a pesticide to control nematodes in agriculture and as an intermediate in pharmaceuticals and fine chemicals manufacture.
- Bis(2-chloroethoxy)methane, also known as Ethane, 1,1'-[methylenebis(oxy)]bis[2-chloro-, is used as a solvent. This chemical may be toxic by ingestion or inhalation and can severely irritates skin, eyes, and mucous membranes.
- 2,4,7,9-Tetramethyl-5-decyn-4,7-diol **(**TMDD), also known by its trade name as Surfynol 104, is classified as a High Production Volume (HPV) chemical. Most of the TMDD manufactured is used as an industrial defoaming, nonionic surfactant. The other uses of TMDD include as an intermediate in the production of polyethylene glycol ether surfactants, in dyes and water-based printing inks applications, and as wetting agent in the formulations of herbicides, fungicides, and insecticides. TMDD has been found to be toxic to aquatic organisms in laboratory experiments on fish (fathead minnows and carp), aquatic invertebrates (*Daphnia magna*), and green algae (*Selenastrum capricornutum)* (US EPA 2001).
- Several representatives of polycyclic aromatic hydrocarbons (PAHs), including fluoranthene, phenanthrene, naphthalene and its derivative tetrahydronaphthalene, naphthalic anhydride, and Anthra-9,10-quinone, which may originate from coal or petroleum. One of the main uses of naphthalene is as an intermediate in the production of phthalic anhydride, which is used then in the production of various materials including phthalate plasticizers, resins, phthaleins, dyes, pharmaceuticals, insect repellents, and others. Tetrahydronaphthalene, also called as tetralin, is used as a solvent. Anthra-9,10-quinone is used mainly as a raw material for dyes manufacture and in some applications in pulp bleaching. In general, the solubility of Anthra-9,10-quinone in water is very low, but it can dissolve in hot solvents, therefore, its presence in the wastewater most likely is the result of high load of solvents in this wastewater that enhanced Anthra-9,10-quinone solubility.

Sample Code	SK170014a	SK17002a	SK17003a	SK17004a	SK17005a	SK17006a	SK17007a	SK17008a
Location	Fortischem							
Number of Compounds Isolated	64	64	75	102	79	82	85	62
Number of Compounds identified to >90%	18	12	12	15	11	12	11	9
Percentage identified to > 90%	28	19	16	15	14	15	13	15
ALKYLATED PHENOLIC COMPOUNDS								
Phenol, 2,3,5-trimethyl-				√				
BENZENE DERIVATIVES								
Benzene, 2-propenyl-	√							
Benzene, 1-propynyl-	√							
1-Naphthalenol, 1,2,3,4-tetrahydro-		√	√	√	√	√	√	
1(2H)-Naphthalenone, 3,4-dihydro-		√	√	√	√	√	√	√
1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propenyl)-	√							
1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-	√							
CHLORINATED COMPOUNDS								
Bis(2-chloroisopropyl) ether	√	√	√	√	√	√	√	√
Propane, 2,2'-oxybis[1-chloro-	√	√	√	√	√	√		√
Methane, bis(2-chloroethoxy)-	√	√	√	√	√	√	√	√
Tris(2-chloroisopropyl)phosphate	√	√						
PHTHALATE ESTERS								
Diethyl phthalate	√		√	√		√		
Diisobutyl phthalate	√							
GLYCOLS & DERIVATIVES								
2-Propanol, 1-(2-methoxypropoxy)-	√							

Table 3: Summary of key organic contaminants present in samples in which sVOCs were identified to >90% reliability.

Sample Code	SK170014a	SK17002a	SK17003a	SK17004a	SK17005a	SK17006a	SK17007a	SK17008a
PAHs & DERIVATIVES								
Fluoranthene				√				
Phenanthrene				√				
Naphthalene	√							
Naphthalene, 1,2,3,4-tetrahydro-	√	√	√	√	√	√	√	√
Naphthalic anhydride				√				
Anthra-9,10-quinone				√				
CARBOXYLIC ACIDS								
Benzoic acid				√				
Dodecanoic acid				√				
ORGANOSULPHUR COMPOUNDS								
Bis-(2-hydroxypropyl)sulfide	√							
OTHERS								
Caffeine	√							
5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104)	√	√	√	√	√	√	√	√
4-Piperidinone, 2,2,6,6-tetramethyl-	√	√	√		√	√	√	√
1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-		√	√				√	
4-Piperidinol, 2,2,6,6-tetramethyl-		√	√		√	√	√	√
4,4'-Azinodi(2,2,6,6-tetramethylpiperidine)		√	√		√	√	√	√
3-Dimethylaminocyclohexanol, cis-					√	√	√	
2,6-Di(t-butyl)-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one (BHT oxidation product)	√							

Table 3 (Cont'd): Summary of key organic contaminants present in samples in which sVOCs were identified to >90% reliability.

- 4-Piperidinone, 2,2,6,6-tetramethyl-, also known as triacetoneamine, is used primarily as a light stabilizer in plastics manufacture and as a starting material in organic synthesis, for example, to produce radical oxydizer 2,2,6,6-tetramethylpiperidine-1-oxyl – (TEMPO) (Ciriminna & Pagliaro 2010).
- 4-Piperidinol, 2,2,6,6-tetramethyl- (Lastar A) is used exclusively as an intermediate in synthesis of light stabilizer 'HALS' (Hindered Amine Light-Stabiliser) for plastics (UNEP 2002).
- Tris(2-chloroisopropyl)phosphate (TCPP) is used in the European Union (EU) as a flame retardant additive for polyurethane. The main use of the treated polyurethane is in rigid foams for construction applications. A smaller but still significant amount is used in flexible foams for furniture. TCPP is one of the main substances to have replaced tris(chloroethyl) phosphate (TCEP) in Europe (ECHA 2008). TCEP is harmful to aquatic organisms (UNEP).

  TCPP is resistant to degradation once released into the environment and, as a result, has been reported as being found in many environmental compartments, with an assumed potential to enter the food chain (van der Veen & de Boer 2012) accumulating predominantly in the marine biota.

A conspicuous feature from the analysis of all of the samples were a series of major peak which could not be identified to any degree of reliability using existing mass-spectral library. Determination of the identity of these compounds would require more detailed forensic analysis using techniques that were beyond the scope of this investigation.

3.2.2 Volatile organic compounds (VOCs)

All of the samples contained a diverse range, and relatively high number, of VOCs (from 47 to 75) and over half of these (60-74%) were reliably identified (see Table 4). The results for quantitative VOCs analysis are presented in Table 5. In general, all halogenated VOCs express toxic properties and some of them are carcinogenic. Of greatest concern in this study was detection of chloroethene, also called as vinyl chloride monomer (VCM), at very high concentrations ranged from 360.4 ± 13.9 to 9419.0 ± 1148.9 µg/l. It should be noted that even these high concentrations could be well underestimated as a result of the high volatility of this compound, which can lead to losses during dilution of the sample that was indispensable step for VCM quantitative analysis.

VCM is among the highest production volume chemicals in the world, with annual worldwide demand of about 7.3 million tonnes (ATSDR 2016). The majority of the VCM produced is used in the production of polyvinyl chloride (PVC) plastic, which is used extensively in construction materials, packaging, electrical and electronic equipment, textiles, coatings, furniture and many other products. Some interest was expressed for the use of PVC in the production of nano-composites (Mamunya *et al.* 2008, Rodríguez-Fernández *et al.* 2008) by adding inorganic nano-scale fillers (Feldman 2014).

VCM itself is highly toxic chemical, with a wide spectrum of toxic effects, including carcinogenicity in both humans and animals, which was recognised many years ago (IARC 1979). VCM is classified as known to be a human carcinogen (DHHS 2014, ATSDR 2016), with the liver being the primary target. A rare type of liver tumor, angiosarcoma, has been strongly associated with occupational exposure to VCM (WHO 2004, DHHS 2014).

Abdominal pain, weakness, fatigue, and weight loss are the most prominent clinical symptoms of VCM poisoning, and hepatosplenomegaly, ascites and jaundice are the most common clinical signs (WHO 2004). Because of its toxicity, VCM has been a subject to many regulations (DHHS 2014), including the US EPA's Clean Air Act, Clean Water Act (Water Quality Criteria: based on fish/shellfish and water consumption - 2 µg/l; based on fish/shellfish only - 530 µg/l) and Safe Water Drinking Act (Maximum Contaminant Level - 2 µg/l). However, the WHO drinking water Quality Guideline Value for VCM is 0.3 µg/l (WHO 2011). Concentrations of VCM in all samples, which could be well underestimated partly because of the loss from its high volatility and sample dilution, exceeded by far all limits mentioned above that is of the great concern in relation to both environmental and human health.

The compound 1,2-dichloroethane, an intermediate in the manufacture of VCM and otherwise known as ethylene dichloride (EDC), was also a conspicuous contaminant in all 8 samples collected in this study. It should be noted that in sample SK17008b, the concentration of 1,2-dichloroethane (504.3 ± 12.6 µg/l) was initially over the calibration range (0.5-400 µg/l). A separate sub-sample of the wastewater collected at this time was diluted 5 times for re-analysis and the calculated concentration was then determined to be 353.0 ± 4.9 µg/l. This difference could very possibly be attributed to the loss during dilution. Both results are reported in Table 5.

Two further chemicals identified in these samples, namely *cis*-1,2-dichloroethene and *trans*-1,2-dichloroethene, are well known by-product contaminants of the wastewaters arising from the production of vinyl chloride, as well as arising from the degradation of other chlorinated solvents such as trichloroethene and tetrachloroethene.

The majority of other chlorinated ethenes, ethanes and methanes detected in the samples, such as 1,1-dichloroethane, trichloroethene, 1,1,2-trichloroethane, & tetrachloroethene are primarily used as solvents and/or as intermediates in the organic synthesis.

A number of trihalomethanes, which can be generated as by-products of water chlorination for disinfection purposes, were also detected in these samples. While some of them were present at trace levels only (Methane, dibromochloro-; methane, bromodichloro- & bromoform), chloroform was found at concentrations ranging from 9.9 (± 0.5) to 229.0 (± 10.2) µg/l. Unless there are deliberate uses of this chemical as a solvent in the industrial processes carried out at the industrial facility, it is possible that it may have been generated unintentionally through reactions occurring as a result of the mixing of other chemical wastes in the treatment process.

Among the other VOCs found at relatively high concentrations in these samples, benzene (from 51.0 ± 2.6 to 140.8 ± 9.6 µg/l) and 1,2-dichloro propane (from 7.8 ± 0.3 to 79.3 ± 2.3 µg/l) have been classified as Group 1 - Carcinogenic to humans by IARC (IARC 2017). 1,2-dichloroethane (from 23.5 ± 2.0 to 504.3 ± 12.6 µg/l), chloroform & tetrachloroethene (detected at a much lower concentration, 2.0 ± 0.1 to 4.3 ± 0.2 µg/l) are listed as "reasonably anticipated to be Human Carcinogens" (ATSDR 2011a,b &c), in addition to other identified toxic effects to human health.

Sample Code	**SK17001b**	**SK17002b**	**SK17003b**	**SK17004b**	**SK17005b**	**SK17006b**	**SK17007b**	**SK17008b**
Location	Fortischem							
Number of Compounds Isolated	47	61	62	61	72	75	73	61
Number of Compounds identified to >90%	34	41	43	41	43	45	45	45
Percentage identified to > 90%	72	67	69	67	60	60	62	74
Chlorinated ethanes & ethenes	11	9	9	11	9	10	9	9
Halogenated methanes	2	6	6	5	6	7	7	7
Benzene & aklylbenzenes	6	6	6	6	7	7	7	6
Chlorinated benzenes	5	5	5	5	5	5	5	5
Aliphatic hydrocarbons & alkyl derivatives	6	5	5	5	5	5	5	7
chlorinated hydrocarbons	x	1	1	1	1	1	1	1
PAHs & derivatives	1	1	2	2	2	2	2	2
Others	3	8	9	6	8	8	9	8

Table 4: Summary of key organic contaminant groups present in samples in which VOCs were identified (to >90% reliability), including an indication of presence for the compounds most commonly identified in these samples, and providing the number of individual compounds where more than one compound was identified for a group.

Sample	SK17001	SK17002	SK17003	SK17004	SK17005	SK17006	SK17007	SK17008
VCM (µg/l)*	360.4±13.9	3815.1±127	4673.1±169.8	8551.3±407.5	5600.2±8.4	5489.4±384.2	6521.0±288.2	9419.0±1148.9
Benzene	140.8 ± 9.6	89.4 ± 2.2	107.6 ± 8.2	69.9 ± 6.5	85.0 ± 4.7	98.8 ± 1.1	107.9	51.0 ± 2.6
Toluene	12.9 ± 0.7	8.7 ± 0.3	14.4 ± 1.0	9.6 ± 0.9	9.9 ± 0.6	11.4 ± 0.2	12.4	11.3 ± 0.6
o-xylene	1.6 ± 0.1	1.5 ± 0.0	2.0 ± 0.1	2.6 ± 0.3	2.5 ± 0.1	2.5 ± 0.0	2.8	2.6 ± 0.1
m- and/or p-xylene	4.4 ± 0.1	11.8 ± 0.5	17.9 ± 1.2	33.9 ± 4.4	30.1 ± 1.8	29.6 ± 0.9	33	33.4 ± 1.6
Benzene, ethyl-	6.4 ± 0.3	6.4 ± 0.3	9.3 ± 0.6	12.4 ± 1.5	12.0 ± 0.8	12.7 ± 0.3	13.8	11.8 ± 0.6
Benzene, isopropyl-	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Cyclohexane	4.9 ± 0.0	3.1 ± 0.1	3.9 ± 0.3	2.8 ± 0.0	3.4 ± 0.1	3.8 ± 0.0	3.7	2.4 ± 0.1
Cyclohexane, methyl-	3.3 ± 0.0	2.5 ± 0.0	2.9 ± 0.1	2.4 ± 0.0	2.6 ± 0.0	2.8 ± 0.0	2.8	2.2 ± 0.0
Carbon disulfide	1.5 ± 0.1	<1.0	<1.0	3.6 ± 0.2	2.3 ± 0.2	1.7 ± 0.1	<1.0	<1.0
Benzene, chloro-	4.6 ± 0.2	2.8 ± 0.0	4.1 ± 0.2	2.8 ± 0.2	3.3 ± 0.2	3.8 ± 0.0	3.8	1.8 ± 0.0
1,2-dichlorobenzene	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
1,3-dichlorobenzene	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
1,4-dichlorobenzene	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
1,2,4-trichlorobenzene	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Methane, dichloro-	N.D.	<1.0	1.2 ± 0.1	N.D.	N.D.	2.0 ± 0.0	1.8	1.7 ± 0.1
Chloroform	9.9 ± 0.5	74.5 ± 3.2	111.4 ± 5.5	197.7 ± 11.9	186.1 ± 6.6	197.5 ± 2.5	195.7	229.0 ± 10.2

Table 5: Concentrations of volatile organic compounds, in µg/l. <xx: < LOQ. N.D. – not detected. The results are presented as average of duplicates ± standard deviation (with the exception for SK17007, for which one of the duplicate subsample vials could not be analyzed)

* signifies that target compound concentration was calculated in diluted sample: by a factor of 100 and 5 for VCM and 1,2-dichloroethane, respectively

Sample	SK17001	SK17002	SK17003	SK17004	SK17005	SK17006	SK17007	SK17008
Methane, bromodichloro-	<1.0	<1.0	<1.0	1.2 ± 0.1	<1.0	<1.0	<1.0	<1.0
Methane, dibromochloro-	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Bromoform	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Methane, tetrachloro-	N.D.	N.D.	N.D.	N.D.	1.1 ± 0.0	1.4 ± 0.0	1.3	1.3 ± 0.0
Ethane, 1,1-dichloro-	6.0 ± 0.2	30.5 ± 0.7	44.5 ± 2.6	82.9 ± 3.2	71.1 ± 2.2	68.9 ± 2.5	76.6	93.0 ± 3.7
Ethane, 1,2-dichloro-	23.5 ± 2.0	116.1 ± 0.4	166.4 ± 10.8	232.5 ± 21.5	221.7 ± 10.6	208.8 ± 8.9	239.3	504.3 ± 12.6 353.0 ± 4.9*
Ethane, 1,1,2-trichloro -	1.2 ± 0.1	1.4 ± 0.0	<1.0	15.2 ± 1.6	58.6 ± 2.5	15.2 ± 0.5	<1.0	<1.0
Ethane, 1,1,2,2-tetrachloro-	N.D.	N.D.	N.D.	2.9 ± 0.4	N.D.	<1.0	N.D.	N.D.
Ethene, 1,1-dichloro-	1.4 ± 0.0	8.2 ± 0.3	12.5 ± 1.1	16.3 ± 0.9	36.4 ± 2.4	18.6 ± 0.1	20.9	28.9 ± 1.6
Ethene, 1,2-dichloro-, cis-	13.0 ± 0.6	15.0 ± 0.4	16.5 ± 1.1	18 ± 1.0	17.7 ± 0.7	19.7 ± 0.8	21.8	23.4 ± 0.8
Ethene, 1,2-dichloro-, trans-	2.0 ± 0.1	2.9 ± 0.1	3.4 ± 0.2	6.4 ± 0.1	5.0 ± 0.2	4.4 ± 0.0	4.5	5.2 ± 0.2
Ethene, trichloro-	10.8 ± 0.5	15.9 ± 0.4	19.9 ± 1.4	28.0 ± 1.8	27.9 ± 1.4	28.6 ± 0.3	31.4	44.6 ± 2.6
Ethene, tetrachloro-	2.0 ± 0.1	2.1 ± 0.1	2.4 ± 0.2	3.4 ± 0.1	3.7 ± 0.2	3.6 ± 0.0	3.5	4.3 ± 0.2
Propane, 1,2-dichloro-	7.8 ± 0.3	24.0 ± 0.3	37.3 ± 2.1	49.3 ± 3.7	47.8 ± 2	47.4 ± 1.8	52.6	79.3 ± 2.3

Table 5 (Cont'd): Concentrations of volatile organic compounds, in µg/l. <xx: < LOQ. N.D. – not detected. The results are presented as average of duplicates ± standard deviation (with the exception for SK17007, for which one of the duplicate subsample vials could not be analysed)

* signifies that target compound concentration was calculated in diluted sample: by a factor of 100 and 5 for VCM and 1,2-dichloroethane, respectively.

The compound cyclohexanamine, N,N-dimethyl- was identified in all samples except SK17004b (which was the highly acidic sample). This chemical is known to be used as catalyst in the manufacture of polyurethane foams, as an intermediate for rubber accelerators and dyes, as well as in the treatment of textiles (Chemtrac, 2017). In the ECHA (European Chemical Agency) classification and labelling information (C&L) inventory database, it has been listed as a flammable liquid and vapour (H226), toxic if swallowed (H301), in contact of skin (H311) and/or if inhaled (H331). It causes severe skin burns and eye damage (H314), and is toxic to aquatic life with long lasting effect (H411) (ECHA 2017). It is also listed in the Catalogue of Hazardous Chemicals of China 2015 (SAWS 2015). Although it was not possible to obtain standards required to quantify this compound, the peak abundance (in qualitative terms) appeared to be far higher than that of VCM in all samples other than SK17004b (in which it was not found) and SK17001b (in which it was present at relatively low abundances compared to other samples). Given the hazards associated with this chemical, the reasons for its presence as such a conspicuous component of the wastewaters regularly discharged from this facility should be investigated and actions taken to prevent its release to the environment.

3.3 24-hour temporal trend of levels of major contaminants in samples

The 24-hour temporal trend of major metals, sVOCs and VOCs are presented in Figures 1, 2 and 3 below, respectively. For metals and VOCs, the concentrations at each sampling time are presented. It should be noted that, in the case of VCM, the concentrations presented in Figure 3 are one tenth of the original VCM concentrations, such that the trends in other VOCs can be viewed on the same axis. In the case of sVOCs, for which only qualitative analysis was carried out, the values shown on the vertical axis are the relative abundance of compounds normalised to the response of an internal standard, which was added to each sample before extraction.

Together, these temporal trends show that the concentrations or relative abundances of major contaminants in the waste water discharge were quite variable over time during the 24h sampling period, with some obvious difference of trends among chemicals. Such trends could be attributed to the difference in the composition and quality of the input waste water (including the changing production status in the industrial facilities), and/or the operation status of the WWTP.

Overall, the presence of highly hazardous chemicals in the treated wastewater samples, especially of extremely high concentrations of mercury and VCM, as well as high peak abundance of N,N-dimethyl-cyclohexanamine, is of great concern and needs urgent further investigations in order to prevent ongoing discharges of contaminants to wider environment.

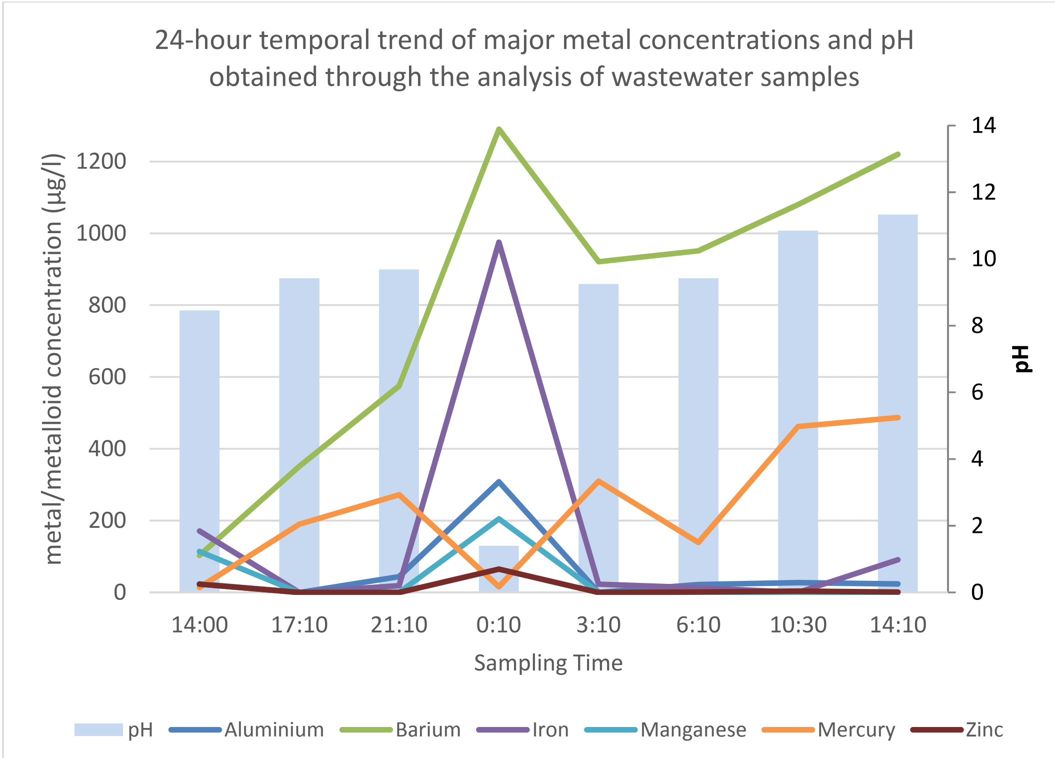
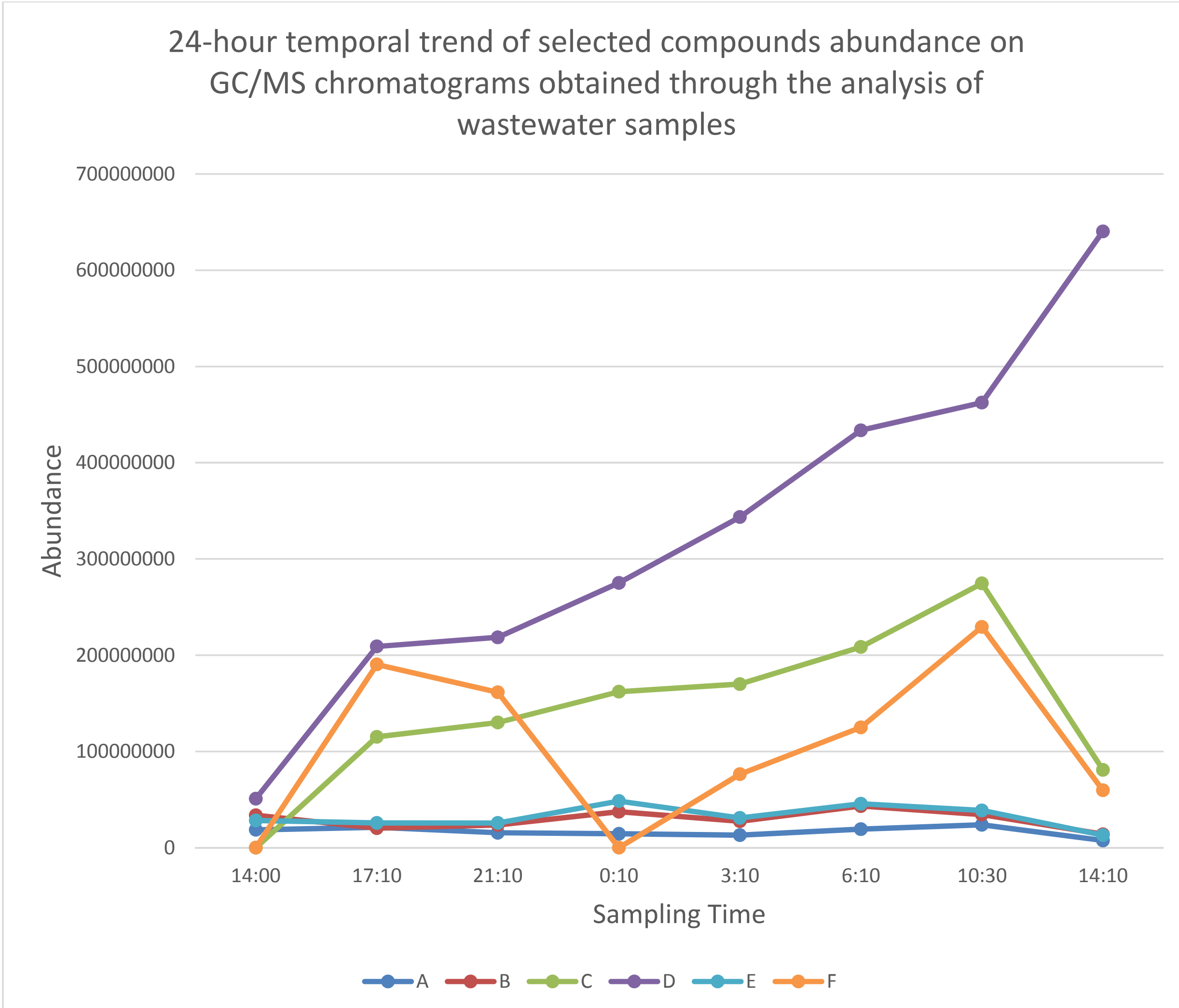
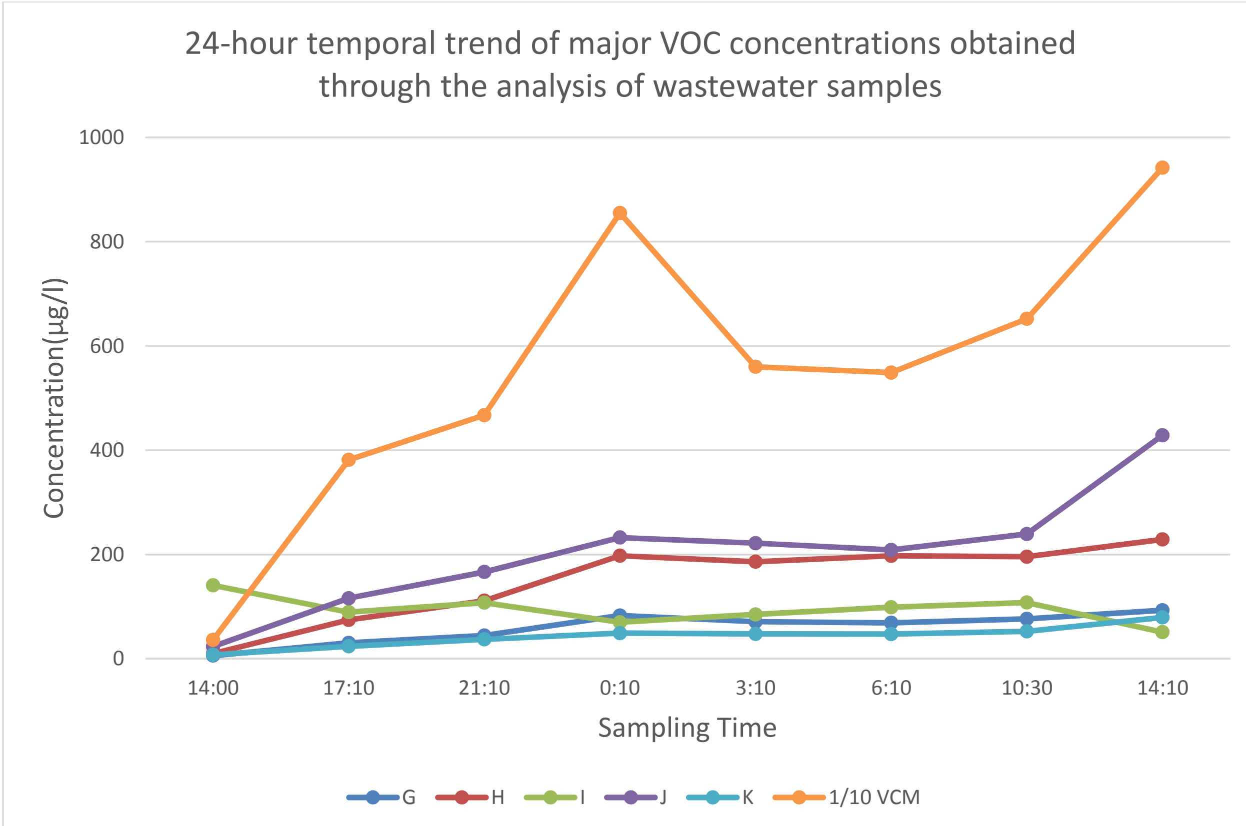


Figure 1. 24-hour temporal trend of concentrations of major metals (coloured lines), and pH (blue bars)



A	Bis(2-chloroisopropyl)ether
B	Methane, bis(2-chloroethoxy)-
C	Unknown
D	Surfynol
E	Chlorinated polyethylene glycol (*tentative identification*)
F	4,4'-Azinodi(2,2,6,6-tetramethylpiperidine)

Figure 2. 24-hour temporal trend of abundance of major sVOCs



G	Ethane, 1,1-dichloro-
H	Chloroform
I	Benzene
J	Ethane, 1,2-dichloro-
K	Propane, 1,2-dichloro-
1/10 VCM	1/10 of VCM concentration

Figure 3. 24-hour temporal trend of concentrations of major VOCs

For more information please contact:

Kevin Brigden, Iryna Labunska, Melissa Wang, David Santillo or Paul Johnston

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Appendix 1: Details of methodologies

Analysis for Volatile Organic Compounds (VOCs)

Methods

VOCs were analysed using an Agilent 7890B gas chromatograph with an Restek Rxi-624Sil column (30m, 0.25mm ID, 1.4µm film thickness) connected to an Agilent 7697A Headspace Sampler and linked to an Agilent 5977A MSD operated in EI mode. The GC oven temperature program included an initial temperature of 43^{0}C (held for 4min), rising to 55^{0}C at 5^{0}C/min, and then to 210^{0}C at 15^{0}C/min (held for 2.5min). The carrier gas was helium, supplied at 1.5ml/min.

From each sample, three 10ml portions were sub-sampled into 20ml headspace vials containing 3g of anhydrous sodium sulfate (analytical reagent grade, with a fourth 20ml headspace vial being filled with the rest of the samples (with no bubble left in the vial)). The first sub-sample was analysed with the GC-MS in total ion monitoring (SCAN) mode to identify as many of the volatile organic compounds present as possible. Identification of compounds was carried out by matching spectra against the Wiley7N Library, employing expert judgment in order to avoid misidentifications. In addition, this sub-sample was also analysed at the same time with the GC-MS in selective ion monitoring (SIM) mode, in order to match the GC-MS spectra obtained against those of mixed standard preparations containing a range of volatile aromatic organic compounds and halogenated alkanes. The two remaining sub-samples were then used for duplicate quantitative analysis for selected halogenated (chlorinated, brominated and mixed) VOCs which had been detected in the samples through screening. If the concentration of certain compounds were over the calibration range, sample in the fourth vial was diluted accordingly for another round of quantification. Quantification was performed in Selective Ion Monitoring (SIM) mode using a multi-point internal calibration method (internal standards: Methane, bromochloro-, 1,2-Dichloroethane-d4, Toluene-d8, and Chlorobenzene-d5). Halogenated VOCs quantified in the water samples with calibration range and limits of quantification (LOQ) are presented in Table 6 below.

Quality control

A number of blanks of laboratory air capped at the time that sub-sampling had taken place were also analysed, alongside samples of the ultra pure reagent water which was used for the preparation of standard calibration solutions. Limits of quantification (LOQ) were defined as the concentration at which the signal to noise ratio (S/N) is 10. The initial calibration curve for each compound of interest was verified immediately prior to sample analysis by analyzing a calibration standard (QC) at a concentration near the midpoint concentration for the calibration range of the GC-MS. For every 10 samples analysed, there was a QC sample being quantified to check the calibration. The relative difference between calculated QC sample concentrations and nominated QC sample concentrations are within ± 25%, apart from 3 compounds: cyclohexane (-38% to -40%), methylcyclohexane (-38% to -40%), and 1,2,4-trichlorobenzen (-36 to -41%)). Further details could be provided upon request.

Compound	Calibration range, µg/L	LOQ, µg/L
VCM	4-640	2
Ethene, 1,1-dichloro-	1-60	0.2
Carbon disulfide		0.07
Methane, dichloro-		0.1
Ethene, 1,2-dichloro-, trans-		0.5
Ethene, 1,2-dichloro-, cis-		0.1
Cyclohexane		0.1
Methane, tetrachloro-		0.1
Ethene, trichloro-		0.03
Cyclohexane, methyl-		0.06
Methane, bromodichloro-		0.1
Toluene		0.06
Ethane, 1,1,2-trichloro -		0.3
Ethene, tetrachloro-		0.03
Methane, dibromochloro-		1.0
Benzene, chloro-		0.03
Benzene, ethyl-		0.04
m- and/or p-xylene		0.02
o-xylene		0.08
Bromoform		1.0
Benzene, isopropyl-		0.02
Ethane, 1122-tetrachloro-		0.1
1,3-dichlorobenzene		0.02
1,4-dichlorobenzene		0.02
1,2-dichlorobenzene		0.01
1,2,4-trichlorobenzene		0.02
Ethane, 1,1-dichloro-	0.5-400	0.1
Chloroform		0.2
Benzene		0.1
Ethane, 1,2-dichloro-		0.5
Propane, 1,2-dichloro-		0.2

Table 6. Limits of Quantification (LOQs) and calibration range for VOCs being quantified.

Analysis for extractable organic compounds

Preparation

20 µg of deuterated naphthalene was added as an Internal Standard (IS) to each portion of sample that was subject to extraction. Water samples (500ml) were prepared using solid phase extraction technique with Dionex AutoTrace workstation, eluting with ethyl acetate followed by a mixture of pentane and toluene (95:5). Obtained extracts were concentrated to a volume of 3ml with a stream of clean nitrogen and cleaned up prior to analysis.

For the clean-up stage, each extract was shaken with 3ml isopropyl alcohol and 3ml TBA-reagent (mixture of 3% tetrabutylammonium hydrogen sulphate and 20% sodium sulphite in deionised water) and left to stand until the aqueous and organic phases had separated. The pentane phase was collected and eluted through a Florisil column, using a 95:5 pentane:toluene mixed eluent, and the cleaned extract concentrated to a final volume of 1ml as before. 20 µg of bromonaphthalene was added to each extract as a second IS prior to GC-MS analysis.

Analysis

For the total organic compounds screening, samples were analysed using an Agilent 6890 Series II GC with Restek Rtx-XLB column (30m, 0.25mm ID, 0.25 µm film thickness) linked to an Agilent 5973 Inert MSD operated in EI mode and interfaced with an Agilent Enhanced Chem Station data system. The GC oven temperature program employed was as follows: an initial temperature of 35^0C, held for 2 minutes, raised to 260^0C at 10^0C/min, then to 320^0C at 6^0C/min (held for 8min). The carrier gas was helium, supplied at 1ml/min. Identification of compounds was carried out by matching spectra against both the Wiley 7N and Pesticides Libraries, using expert judgment as necessary in order to avoid misidentifications. Additionally, both the spectra and retention times of compounds isolated from the samples were matched against those obtained during GC-MS analysis of standard mixtures containing a range of chlorinated benzenes, phenols and pesticides, polychlorinated biphenyls (PCBs), phthalates, polycyclic aromatic hydrocarbons (PAHs) and aliphatic hydrocarbons.

Quality control

A number of extraction and solvent blanks were also analysed to ensure the detection of any possible contamination resulting from sample handling in the laboratory. Any background contaminants detected in blanks are subtracted from the chromatograms obtained for the samples before mass spectra are interpreted.

Analysis for metals

Preparation

A portion of each whole sample was filtered through a 0.45 micron filter and then acidified by the addition of concentrated nitric acid to give a final concentration of 5% v/v, to enable determination of dissolved metal concentrations. 25 ml of each acidified sample was digested firstly overnight at room temperature, then using microwave-assisted digestion with a CEM MARS Xpress system, with a temperature ramp to 180°C over 15 minutes followed by holding at 180°C for a further 15 minutes. Cooled digests were filtered and made up to 25 ml with deionised water.

Analysis

Prepared sample digests were analysed by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) using an Agilent 7900 Spectrometer utilizing a collision cell with helium as the collision gas to minimize polyatomic interferences. Multi-element standards, matrix matched to the samples, at concentrations of 1, 10, 100 and 1000 μg/l respectively, other than for mercury (0.5, 2, 5, 20 μg/l respectively) were used for instrument calibration. Analysis employed in-line addition of an internal standard mix at 1000 μg/l (Scandium, Germanium, Yttrium, Indium and Terbium).

Quality control

One sample was prepared for ICP analysis in duplicate and analysed to verify method reproducibility, along with a blank sample. Two mixed metal quality control solution of 80 and 800 μg/l for each metal, other than mercury at 4 and 16 μg/l, were digested and analysed. All control samples were prepared in an identical manor to the samples.

Calibration of the ICP-MS was validated by the use of quality control standards at 80 μg/l and 800 μg/l (4 μg/l and 16 μg/l for mercury) prepared in an identical manner but from different reagent stocks to the instrument calibration standards.

pH analysis

The pH of each sample was determined using a Hanna Instruments HI98129 pH meter calibrated using pH 4.01, pH 7.01 and pH 10.01 Hanna buffer solutions. The pH meter and electrode was rinsed will with deionised water between samples.

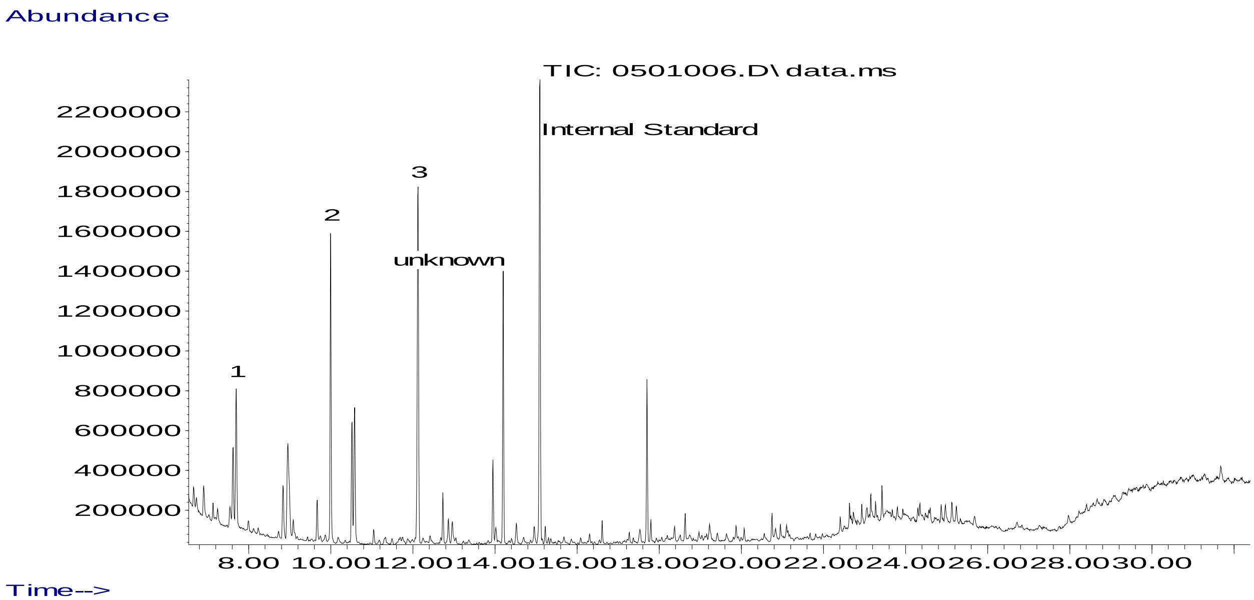
Further details of the methods employed can be provided on request.

Appendix 2: Detailed semi-volatile organic and volatile organic analytical screening data

Detailed screening data arising from GC-MS analysis of each of the samples are presented below. These data list separately semi-volatile organic compounds (SVOCs) identified following solvent extraction and volatile organic compounds (VOCs) identified through separate headspace GC-MS analysis. Only those substances identified to greater than 90% quality match (following verification by expert interpretation) are listed here.

Semi-volatile organic analysis results

Sample code	SK17001a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	14:00 21.02.2017
Description	Wastewater discharge



Number of compounds isolated: 64

Compounds identified to better than 90%:

CAS# **Name**

000084-66-2 1,2-Benzenedicarboxylic acid, diethyl ester

000084-69-5 1,2-Benzenedicarboxylic acid, diisobutyl ester

000523-80-8 1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propenyl)-

006803-02-7 1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-

010396-80-2 2,6-Di(t-butyl)-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one *(BHT oxidation product)*

013429-07-7 2-Propanol, 1-(2-methoxypropoxy)-

000826-36-8 4-Piperidinone, 2,2,6,6-tetramethyl-

000126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 3*]**

000673-32-5 Benzene, 1-propynyl-

000300-57-2 Benzene, 2-propenyl-

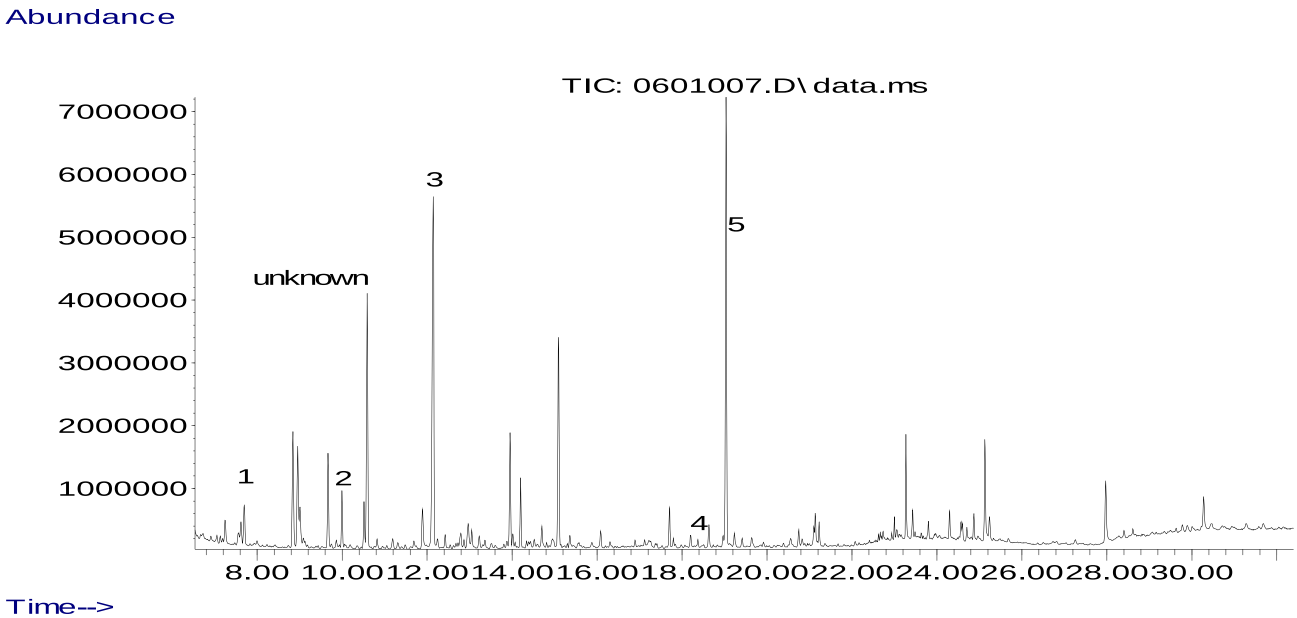
039638-32-9 Bis(2-chloroisopropyl) ether **[*Compound 1*]**

006704-15-0 Bis-(2-hydroxypropyl)sulfide

000058-08-2	Caffeine
000111-91-1	Methane, bis(2-chloroethoxy)- **[*Compound 2*]**
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000108-60-1	Propane, 2,2'-oxybis[1-chloro-
013674-84-5	Tris(2-chloroisopropyl)phosphate

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17002a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	17:10 21.02.2017
Description	Wastewater discharge



Number of compounds isolated: 64

Compounds identified to better than 90%:

CAS# **Name**

000529-34-0 1(2H)-naphthalenone, 3,4-dihydro-

000529-33-9 1-Naphthalenol, 1,2,3,4-tetrahydro-

002226-96-2 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-

018528-42-2 4,4'-Azinodi(2,2,6,6-tetramethylpiperidine)
[*Compound 5*]

002403-88-5 4-Piperidinol, 2,2,6,6-tetramethyl-

000826-36-8 4-Piperidinone, 2,2,6,6-tetramethyl-

000126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104)
[*Compound 3*]

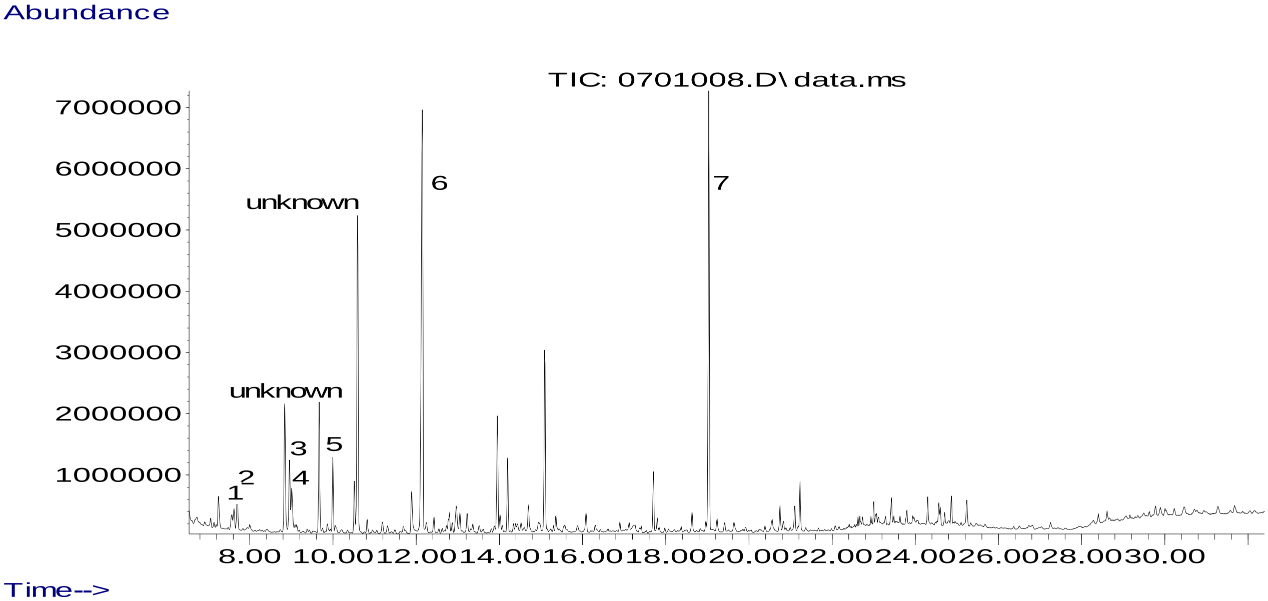
039638-32-9 Bis(2-chloroisopropyl) ether
[*Compound 1*]

000111-91-1 Methane, bis(2-chloroethoxy)-
[*Compound 2*]

000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000108-60-1	Propane, 2,2'-oxybis[1-chloro-
013674-84-5	Tris(2-chloroisopropyl)phosphate **[*Compound 4*]**

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17003a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	21:10 21.02.2017
Description	Wastewater discharge



Number of compounds isolated: 75

Compounds identified to better than 90%:

CAS# **Name**

000529-34-0 1(2H)-Naphthalenone, 3,4-dihydro-

000084-66-2 1,2-Benzenedicarboxylic acid, diethyl ester

000529-33-9 1-Naphthalenol, 1,2,3,4-tetrahydro-

002226-96-2 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-

018528-42-2 4,4'-Azinodi(2,2,6,6-tetramethylpiperidine)
[*Compound 7*]

002403-88-5 4-Piperidinol, 2,2,6,6-tetramethyl-
[*Compound 4*]

000826-36-8 4-Piperidinone, 2,2,6,6-tetramethyl-
[*Compound 3*]

000126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104)
[*Compound 6*]

039638-32-9 Bis(2-chloroisopropyl) ether
[*Compound 2*]

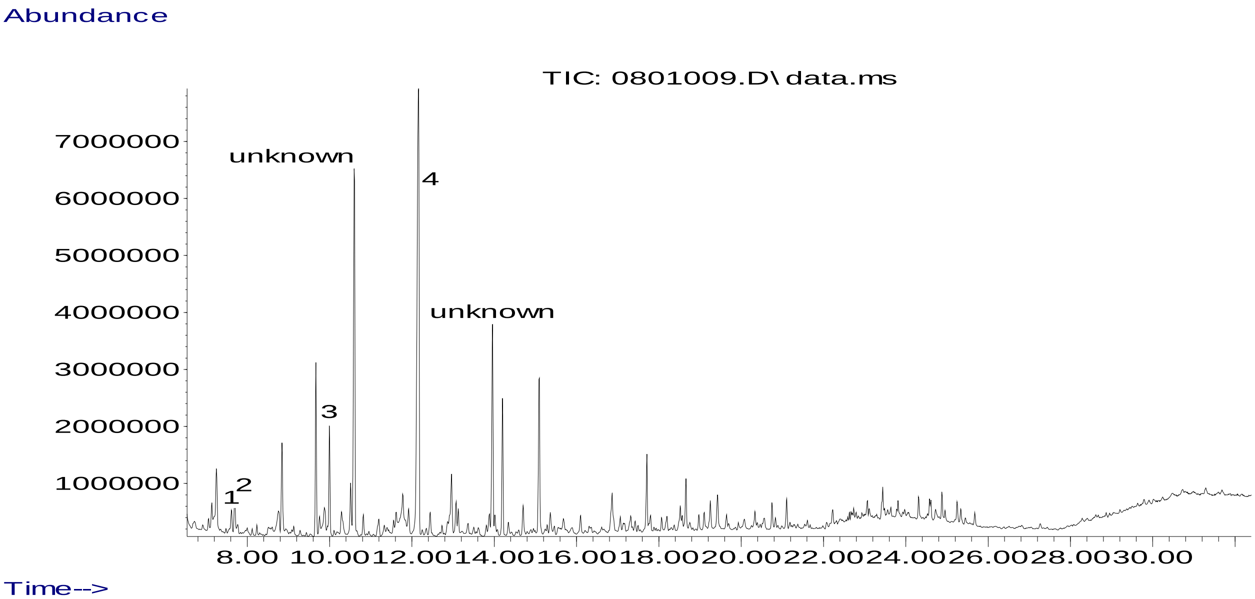
000111-91-1 Methane, bis(2-chloroethoxy)-
[*Compound 5*]

000119-64-2 Naphthalene, 1,2,3,4-tetrahydro-

000108-60-1 Propane, 2,2'-oxybis[1-chloro-
[*Compound 1*]

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17004a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	00:10 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: 102

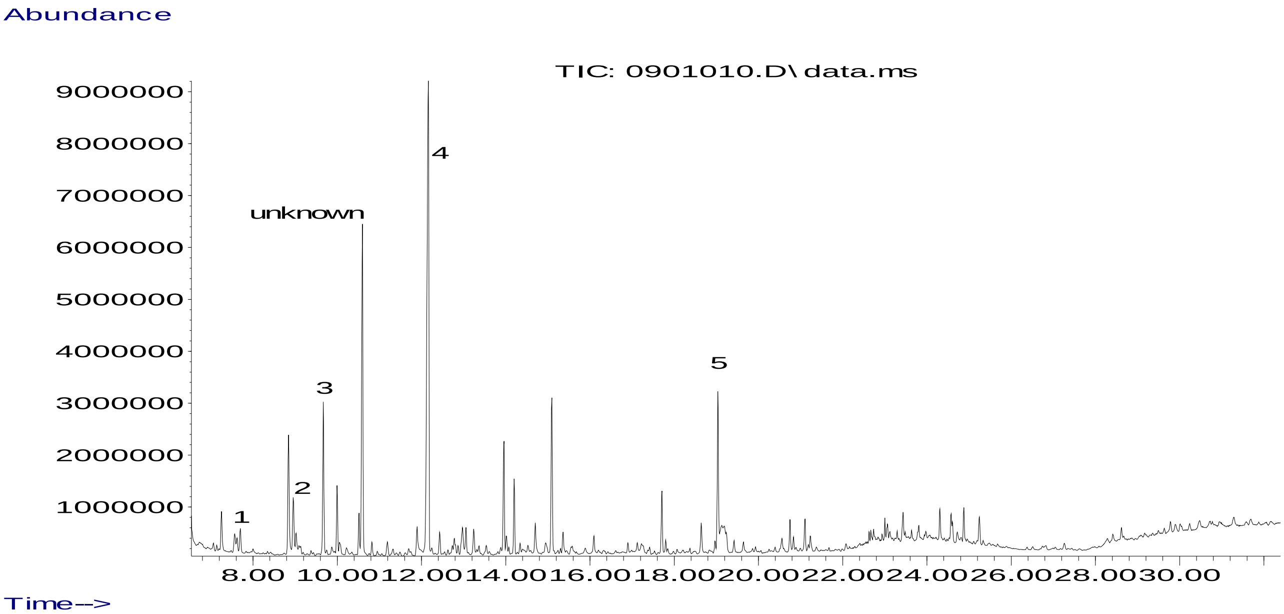
Compounds identified to better than 90%:

CAS#	**Name**
000084-66-2	1,2-Benzenedicarboxylic acid, diethyl ester
000529-34-0	1(2H)-Naphthalenone, 3,4-dihydro-
000529-33-9	1-Naphthalenol, 1,2,3,4-tetrahydro-
000126-86-3	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 4*]**
000084-65-1	Anthra-9,10-quinone
000065-85-0	Benzoic acid
039638-32-9	Bis(2-chloroisopropyl) ether **[*Compound 2*]**
000143-07-7	Dodecanoic acid
000206-44-0	Fluoranthene
000111-91-1	Methane, bis(2-chloroethoxy)- **[*Compound 3*]**

000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000081-84-5	Naphthalic anhydride
000085-01-8	Phenanthrene
000697-82-5	Phenol, 2,3,5-trimethyl-
000108-60-1	Propane, 2,2'-oxybis[1-chloro- **[*Compound 1*]**

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17005a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	03:10 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: 79

Compounds identified to better than 90%:

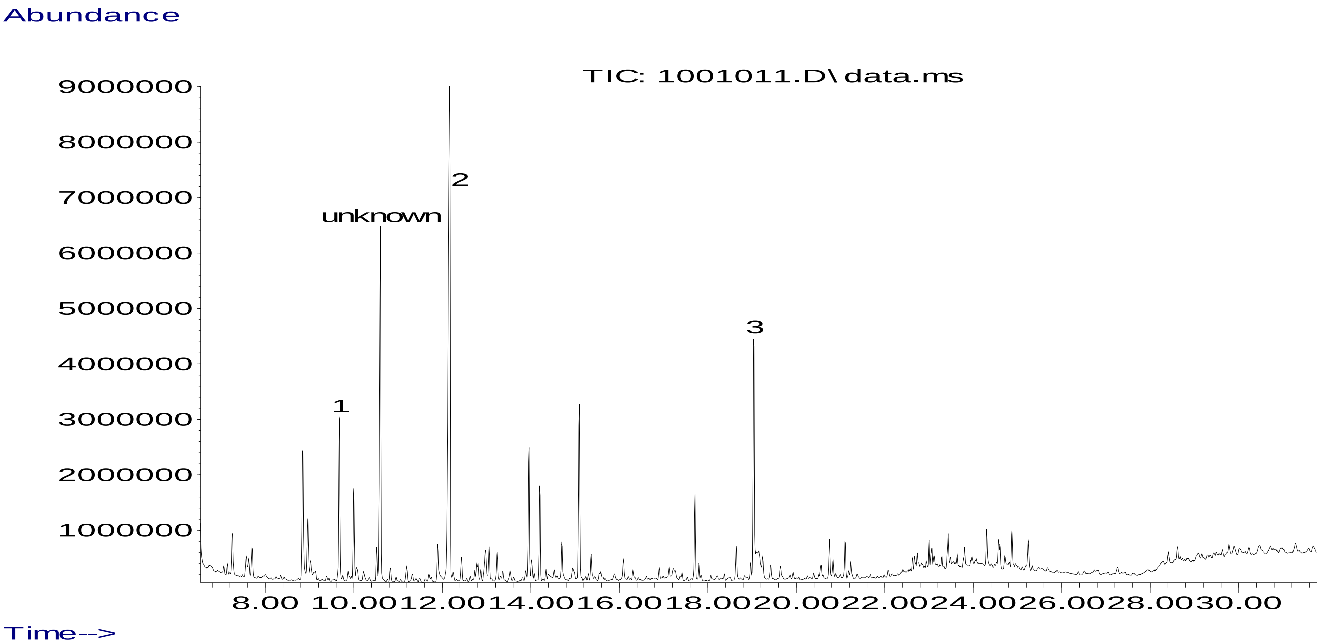
CAS#	**Name**
000529-34-0	1(2H)-Naphthalenone, 3,4-dihydro-
000529-33-9	1-Naphthalenol, 1,2,3,4-tetrahydro-
006982-36-1	3-Dimethylaminocyclohexanol, cis-
018528-42-2	4,4'-Azinodi(2,2,6,6-tetramethylpiperidine) **[*Compound 5*]**
002403-88-5	4-Piperidinol, 2,2,6,6-tetramethyl-
000826-36-8	4-Piperidinone, 2,2,6,6-tetramethyl- **[*Compound 2*]**
000126-86-3	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 4*]**
000111-91-1	Methane, bis(2-chloroethoxy)-
039638-32-9	Bis(2-chloroisopropyl) ether **[*Compound 1*]**

000119-64-2 Naphthalene, 1,2,3,4-tetrahydro-
[*Compound 3*]

000108-60-1 Propane, 2,2'-oxybis[1-chloro-

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17006a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	06:10 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: **82**

Compounds identified to better than 90%:

CAS# **Name**

000084-66-2 1,2-Benzenedicarboxylic acid, diethyl ester

000529-34-0 1(2H)-Naphthalenone, 3,4-dihydro-

000529-33-9 1-Naphthalenol, 1,2,3,4-tetrahydro-

006982-36-1 3-Dimethylaminocyclohexanol, cis-

018528-42-2 4,4'-Azinodi(2,2,6,6-tetramethylpiperidine) **[*Compound 3*]**

002403-88-5 4-Piperidinol, 2,2,6,6-tetramethyl-

000826-36-8 4-Piperidinone, 2,2,6,6-tetramethyl-

000126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 2*]**

039638-32-9 Bis(2-chloroisopropyl) ether

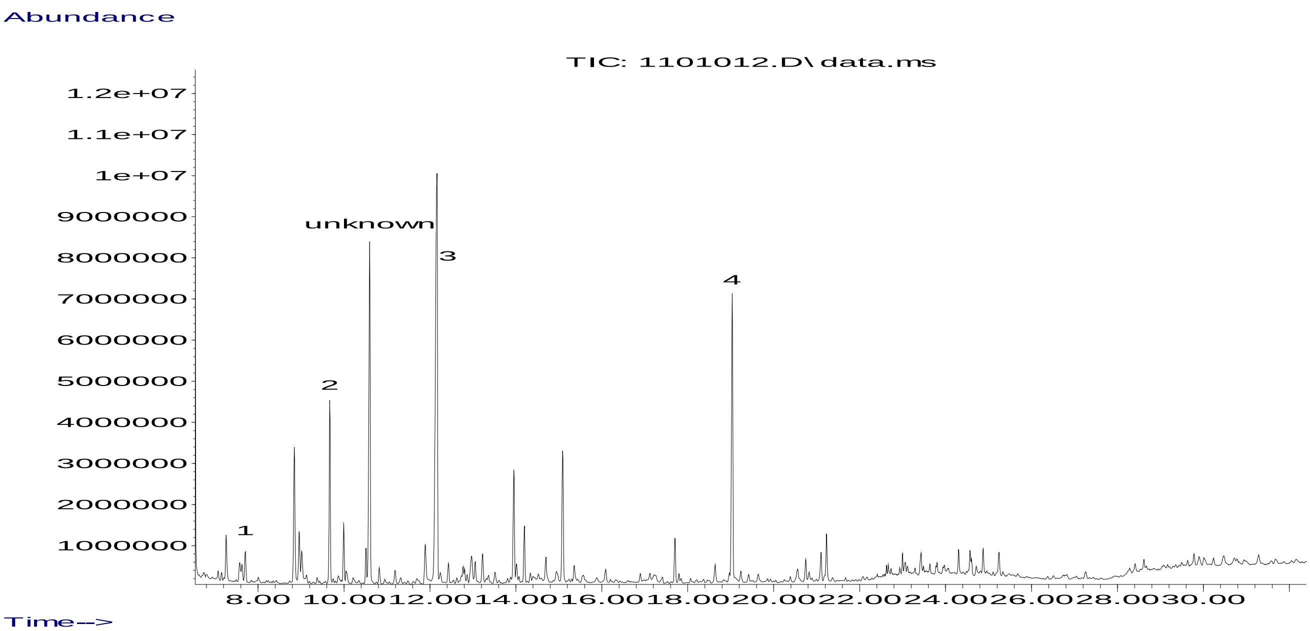
000111-91-1 Methane, bis(2-chloroethoxy)-

000119-64-2 Naphthalene, 1,2,3,4-tetrahydro-
[*Compound 1*]

000108-60-1 Propane, 2,2'-oxybis[1-chloro-

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17007a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	10:30 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: 85

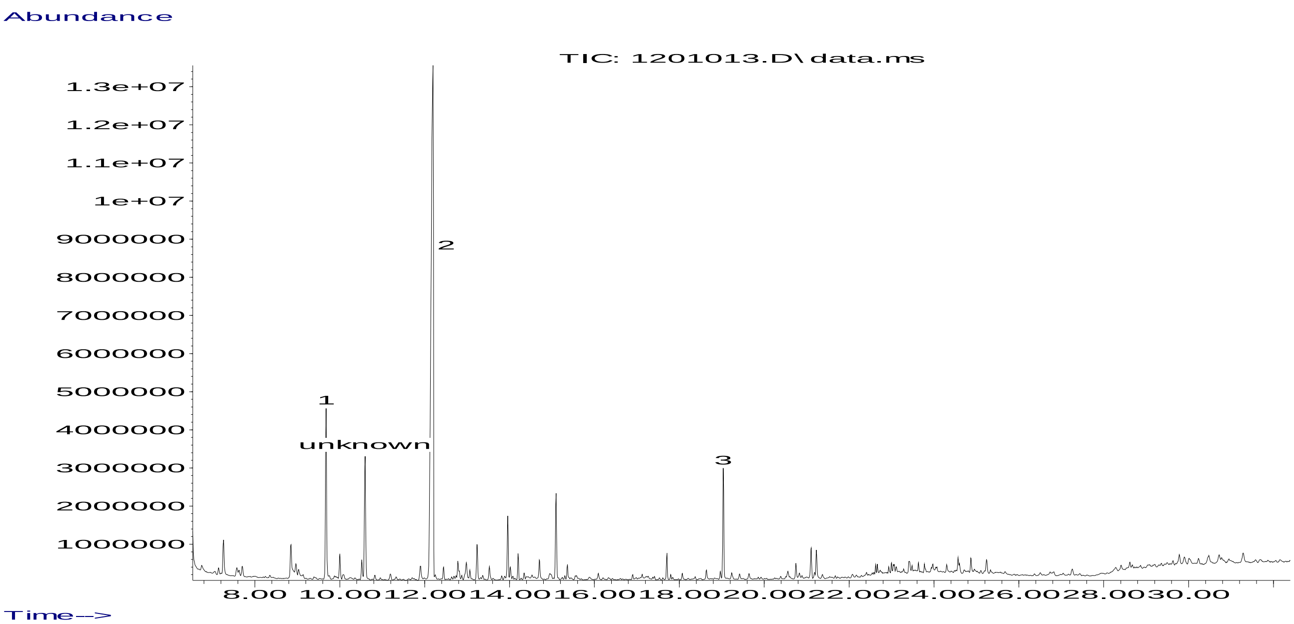
Compounds identified to better than 90%:

CAS#	**Name**
000529-34-0	1(2H)-Naphthalenone, 3,4-dihydro-
000529-33-9	1-Naphthalenol, 1,2,3,4-tetrahydro-
002226-96-2	1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-
006982-36-1	3-Dimethylaminocyclohexanol, cis-
018528-42-2	4,4'-Azinodi(2,2,6,6-tetramethylpiperidine) **[*Compound 4*]**
002403-88-5	4-Piperidinol, 2,2,6,6-tetramethyl-
000826-36-8	4-Piperidinone, 2,2,6,6-tetramethyl-
000126-86-3	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 3*]**
039638-32-9	Bis(2-chloroisopropyl) ether **[*Compound 1*]**
000111-91-1	Methane, bis(2-chloroethoxy)-

000119-64-2 Naphthalene, 1,2,3,4-tetrahydro-
[*Compound 2*]

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Sample code	SK17008a
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	14:10 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: 62

Compounds identified to better than 90%:

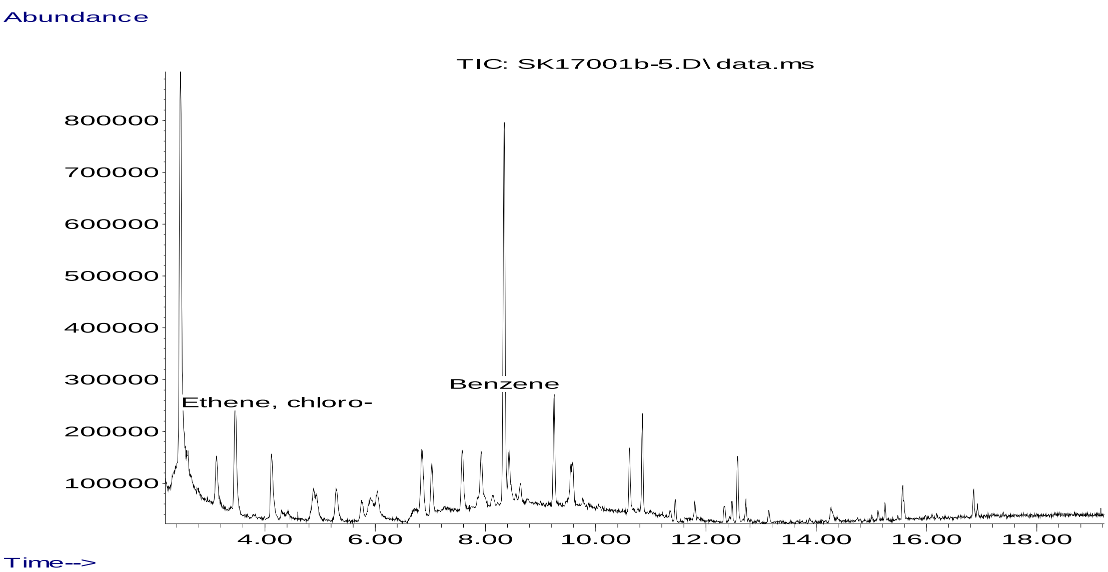
CAS#	**Name**
000529-34-0	1(2H)-Naphthalenone, 3,4-dihydro-
018528-42-2	4,4'-Azinodi(2,2,6,6-tetramethylpiperidine) **[*Compound 3*]**
002403-88-5	4-Piperidinol, 2,2,6,6-tetramethyl-
000826-36-8	4-Piperidinone, 2,2,6,6-tetramethyl-
000126-86-3	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (synonym: Surfynol 104) **[*Compound 2*]**
039638-32-9	Bis(2-chloroisopropyl) ether
000111-91-1	Methane, bis(2-chloroethoxy)-
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro- **[*Compound 1*]**
000108-60-1	Propane, 2,2'-oxybis[1-chloro-

Note: chromatogram contained a number of compounds, including chlorinated compounds, that could not be reliably identified. Some of them have shown GC/MS fragmentation similar to that of chlorinated polyethylene glycols.

Volatile organic analysis results

Note: Some compounds have been identified only at trace levels using Selective Ion Monitoring (SIM) method, which is indicated below next to the name of the such compound.

Sample code	SK17001b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	14:00 21.02.2017
Description	Wastewater discharge



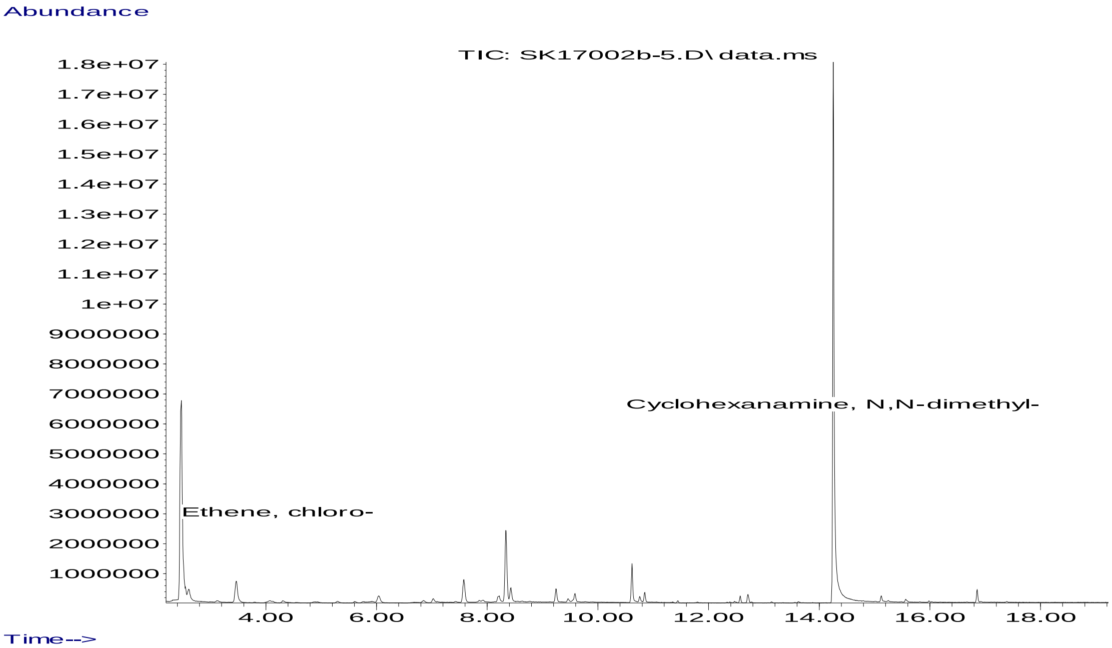
Number of compounds isolated: 47

Compounds identified to better than 90%: 34

CAS#	**Name**
000000-00-0	2-Pentanone, methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000078-78-4	Butane, 2-methyl-
000067-66-3	Chloroform
000098-94-2	Cyclohexanamine, n,n-dimethyl-
000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-

000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000079-00-5	Ethane, 1,1,2-trichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p-xylene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000075-15-0	Carbon disulfide (SIM)
000075-35-4	Ethene, 1,1-dichloro- (SIM)
000156-60-5	Ethene, 1,2-dichloro-, trans- (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)

Sample code	SK17002b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	17:10 21.02.2017
Description	Wastewater discharge



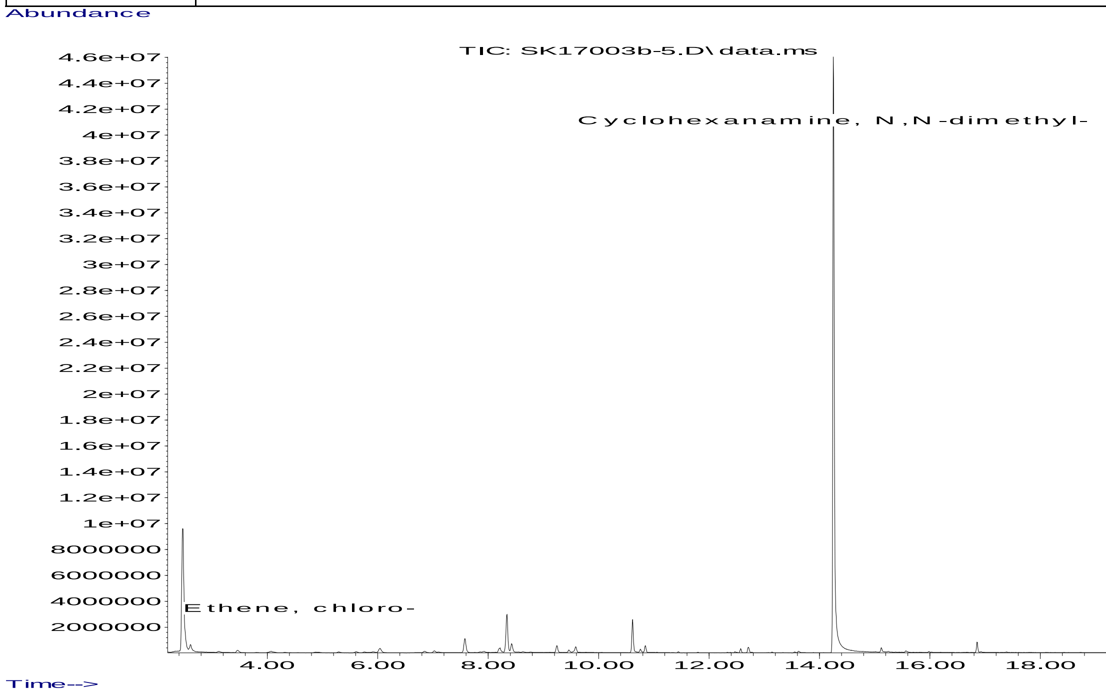
Number of compounds isolated: 61

Compounds identified to better than 90%: 41

CAS#	**Name**
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000078-78-4	Butane, 2-methyl-
000000-00-0	Butanal or Propanal, methyl- (2 isomers)
000075-15-0	Carbon disulfide
000098-94-2	Cyclohexanamine, n,n-dimethyl-
000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-

000079-00-5	Ethane, 1,1,2-trichloro-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-60-5	Ethene, 1,2-dichloro-, trans-
000156-59-2	Ethene, 1,2-dichloro-,cis
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000067-66-3	Methane, trichloro- (chloroform)
000091-20-3	Naphthalene
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000123-38-6	Propanal
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000075-09-2	Methane, dichloro- (SIM)

Sample code	SK17003b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	21:10 21.02.2017
Description	Wastewater discharge



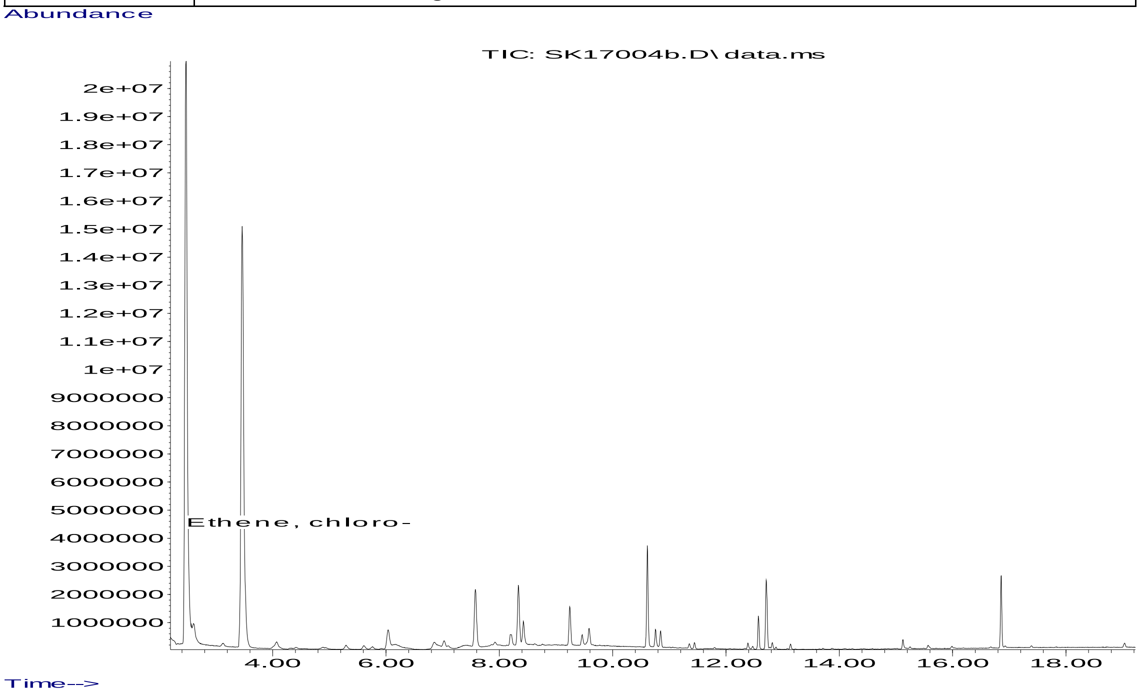
Number of compounds isolated: 62

Compounds identified to better than 90%: 43

CAS#	**Name**
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000078-85-3	2-Propenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-

000067-66-3	Chloroform
000098-94-2	Cyclohexanamine, n,n-dimethyl-
000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis-
000156-60-5	Ethene, 1,2-dichloro-, trans-
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p- xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000075-15-0	Carbon disulfide (SIM)
000079-00-5	Ethane, 1,1,2-trichloro- (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000075-09-2	Methane, dichloro- (SIM)

Sample code	SK17004b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	00:10 22.02.2017
Description	Wastewater discharge



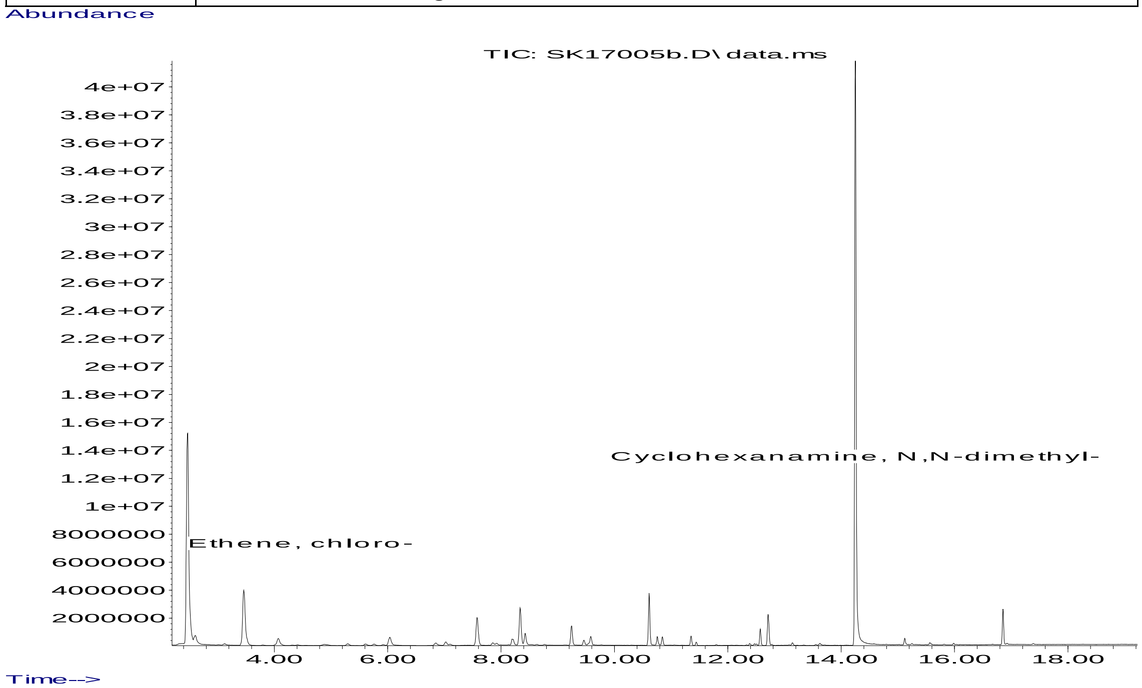
Number of compounds isolated: 61

Compounds identified to better than 90%: 41

CAS#	**Name**
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-
000075-15-0	Carbon disulfide
000067-66-3	Chloroform

000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000079-34-5	Ethane, 1,1,2,2-tetrachloro-
000079-00-5	Ethane, 1,1,2-trichloro-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000683-53-4	Ethane, 2-bromo-1,1-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000156-60-5	Ethene, 1,2-dichloro-, trans-
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000078-87-5	Propane, 1,2-dichloro-
000107-83-5	Propane, 2-methyl-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)

Sample code	SK17005b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	03:10 22.02.2017
Description	Wastewater discharge



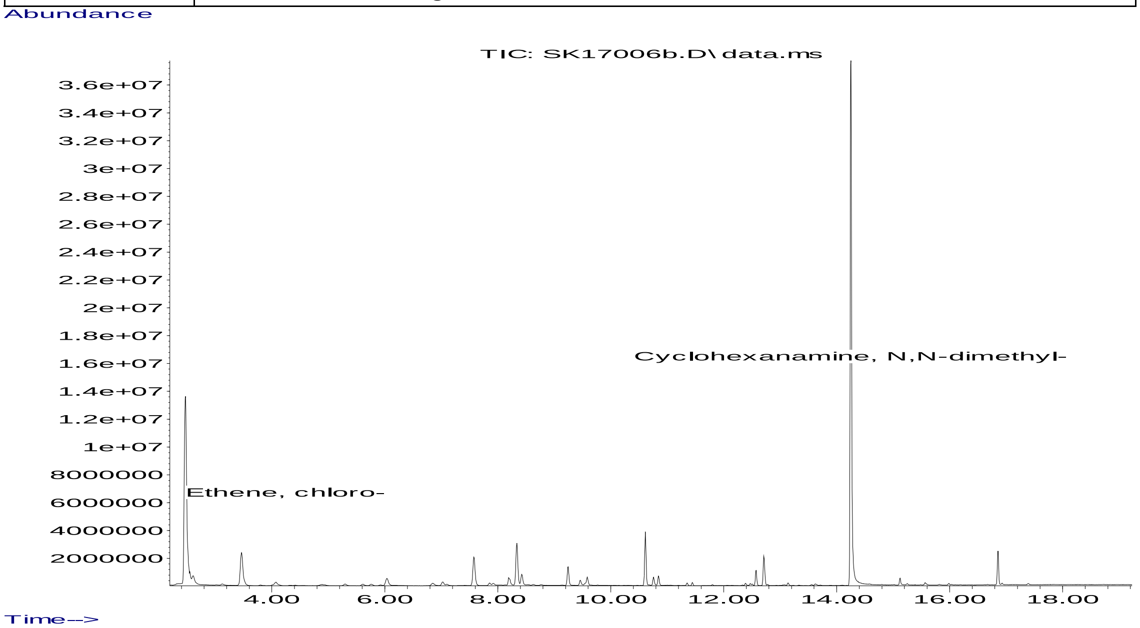
Number of compounds isolated: 72

Compounds identified to better than 90%: 43

CAS#	Name
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-
000075-15-0	Carbon disulfide
000098-94-2	Cyclohexanamine, n,n-dimethyl-

000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000079-00-5	Ethane, 1,1,2-trichloro-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000156-60-5	Ethene, 1,2-dichloro-, trans-
000075-01-4	Ethene, chloro-
000079-01-6	Ethene, trichloro-
000127-18-4	Ethene, tetrachloro-
000110-54-3	Hexane
000095-13-6	Indene
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000067-66-3	Methane, trichloro- (Chloroform)
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000056-23-5	Methane, tetrachloro- (SIM)

Sample code	SK17006b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	06:10 22.02.2017
Description	Wastewater discharge



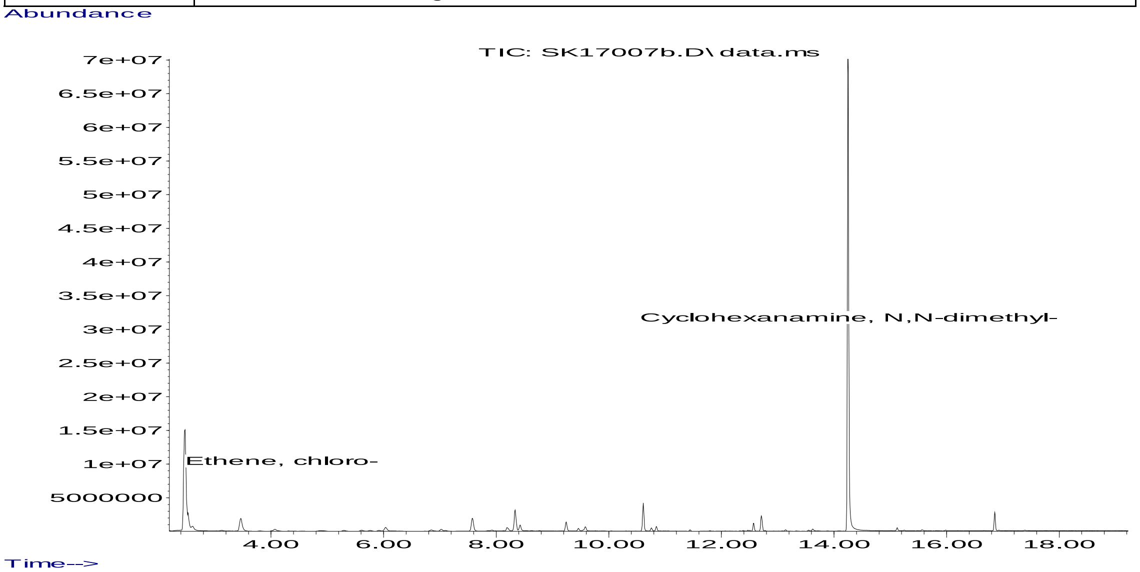
Number of compounds isolated: 75

Compounds identified to better than 90%: 45

CAS#	Name
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000095-13-6	1H-indene
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000098-82-8	Benzene, isopropyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-
000075-15-0	Carbon disulfide

000098-94-2	Cyclohexanamine, n,n-dimethyl-
000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000079-00-5	Ethane, 1,1,2-trichloro-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000156-60-5	Ethene, 1,2-dichloro-, trans
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000067-66-3	Methane, trichloro- (Chloroform)
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000075-25-2	Bromoform (SIM)
000079-34-5	Ethane, 1,1,2,2-tetrachloro- (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000075-09-2	Methane, dichloro- (SIM)
000056-23-5	Methane, tetrachloro- (SIM)

Sample code	SK17007b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	10:30 22.02.2017
Description	Wastewater discharge



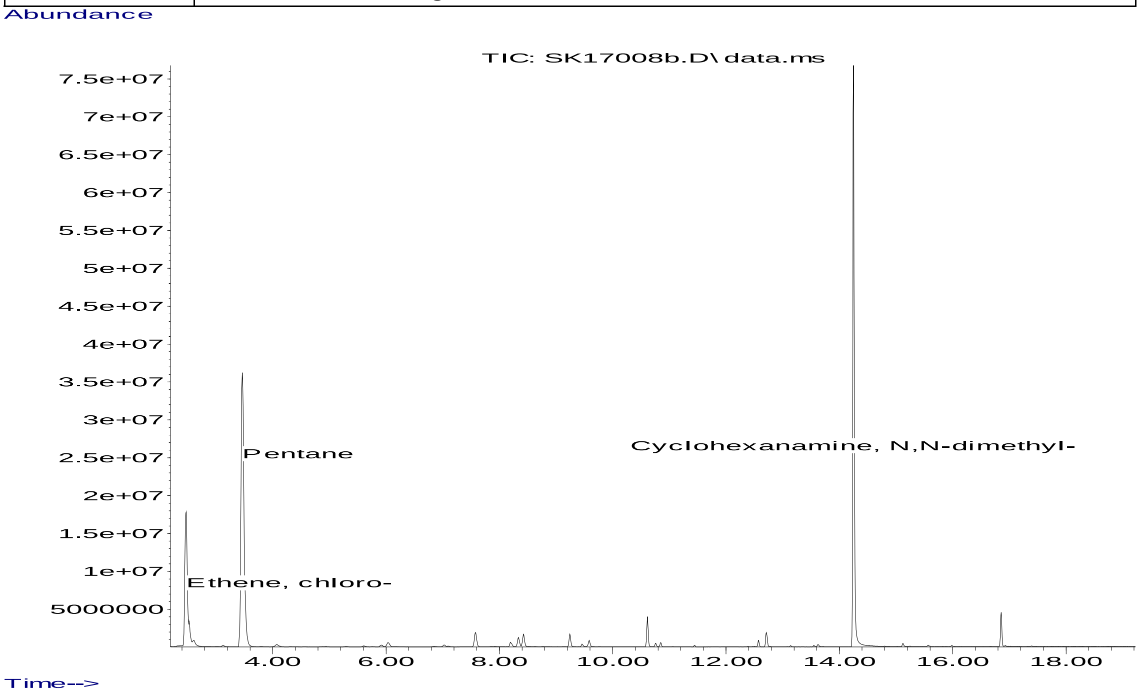
Number of compounds isolated: 73

Compounds identified to better than 90%: 45

CAS#	**Name**
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000095-13-6	1H-indene
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000078-85-3	2-Propenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-
000075-15-0	Carbon disulfide
000098-94-2	Cyclohexanamine, n,n-dimethyl-

000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000156-60-5	Ethene, 1,2-dichloro-, trans
000075-01-4	Ethene, chloro-
000127-18-4	Ethene, tetrachloro-
000079-01-6	Ethene, trichloro-
000110-54-3	Hexane
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000075-09-2	Methane, dichloro-
000067-66-3	Methane, trichloro- (Chloroform)
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000079-00-5	Ethane, 1,1,2-trichloro- (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000056-23-5	Methane, tetrachloro- (SIM)

Sample code	SK17008b
Location	Fortischem, a. s. Industrial site, Nováky town, District of Prievidza city, Slovakia
Sample type	Treated wastewater
Date & time	14:10 22.02.2017
Description	Wastewater discharge



Number of compounds isolated: 61

Compounds identified to better than 90%: 45

CAS#	Name
000000-00-0	1-Propanol, 2-methyl- or 2-butanol
000000-00-0	2-Butenal, methyl-
000000-00-0	2-Pentanone, methyl-
000623-36-9	2-Pentenal, 2-methyl-
000078-85-3	2-Propenal, 2-methyl-
000071-43-2	Benzene
000108-90-7	Benzene, chloro-
000100-41-4	Benzene, ethyl-
000000-00-0	Butanal or propanal, 2-methyl-
000078-78-4	Butane, 2-methyl-
000075-15-0	Carbon disulfide

000098-94-2	Cyclohexanamine, n,n-dimethyl-
000110-82-7	Cyclohexane
000108-87-2	Cyclohexane, methyl-
000075-34-3	Ethane, 1,1-dichloro-
000107-06-2	Ethane, 1,2-dichloro-
000075-35-4	Ethene, 1,1-dichloro-
000156-59-2	Ethene, 1,2-dichloro-, cis
000156-60-5	Ethene, 1,2-dichloro-, trans
000075-01-4	Ethene, chloro-
000079-01-6	Ethene, trichloro-
000127-18-4	Ethene, tetrachloro-
000000-00-0	M- and/or p-xylene
000111-91-1	Methane, bis(2-chloroethoxy)-
000067-66-3	Methane, trichloro- (Chloroform)
000110-54-3	N-hexane
000091-20-3	Naphthalene
000119-64-2	Naphthalene, 1,2,3,4-tetrahydro-
000095-47-6	O-xylene
000109-66-0	Pentane
000107-83-5	Pentane, 2-methyl-
000768-66-1	Piperidine, 2,2,6,6-tetramethyl-
000078-87-5	Propane, 1,2-dichloro-
000108-88-3	Toluene
000095-50-1	Benzene, 1,2-dichloro- (SIM)
000541-73-1	Benzene, 1,3-dichloro- (SIM)
000106-46-7	Benzene, 1,4-dichloro- (SIM)
000120-82-1	Benzene, 1,2,4-trichloro- (SIM)
000098-82-8	Benzene, isopropyl- (SIM)
000075-25-2	Bromoform (SIM)
000079-00-5	Ethane, 1,1,2-trichloro- (SIM)
000075-27-4	Methane, bromodichloro- (SIM)
000124-48-1	Methane, dibromochloro- (SIM)
000075-09-2	Methane, dichloro- (SIM)
000056-23-5	Methane, tetrachloro- (SIM)