



# Unknown and new organic pollutants in the MULTISOURCE ENTS pilots

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## EXECUTIVE SUMMARY

This document reports on the work carried out in MULTISOURCE *Task 2.1 - Non-target screening of unknown and new pollutants and microplastics in pilots*, regarding the suspect screening of hazardous chemicals. It specifically addresses *WP2 - Risk Assessment* specific objective to identify unknown and new hazardous organic chemicals in the Enhanced Natural Treatment Solutions pilots (ENTS pilots).

Aarhus University analyzed samples from all seven MULTISOURCE technical pilots (inlets from all sites, and outlets from the pilots in Belgium, Italy, Norway and Germany). This included a complementary analytical approach using high-resolution mass spectrometry after chromatographic separation by liquid-chromatography and gas-chromatography. The samples were injected directly in a UHPLC-QTOF, while for the GC-Orbitrap analysis samples were prepared by liquid-liquid extraction. Samples were acquired using data-dependent acquisition modes on both instruments. A suspect-screening workflow was employed by using instrument proprietary software together with own library (MULTISOURCE Suspect List), proprietary libraries (Sciex, NIST), as well as an online database (MassBank).

Results include 3708 features by GC-Orbitrap and up to 4000 features by UHPLC-QTOF analysis, which after software supported filtration resulted in a combined list of 181 identified compounds. From these identified compounds, 27 are already included in the target methods and 10 compounds were part of the MULTISOURCE suspect list, while 144 compounds were retrieved from the other databases. Out of the 181 identified compounds, 147 compounds were found up to 4 times in different samples, while 34 compounds were found frequently ( $\geq 5$  times).

At this stage it is recommended the inclusion of the following compounds on the MULTISOURCE target methods:

LC-MS/MS: strychnine, guanosine, indoxyl, acetaminophen, 2'-deoxyguanosine, naproxen, perfluoropropane sulfonamido propyl dimethyl quaternary amine propanoate, hydroxyethylflurazepam and N-Desmethyl-cis-tramadol.

GC-MS: tris(1-chloro-2-propyl) phosphate, 2-(methylthio)benzothiazole, benzophenone, triphenyl phosphate, tris(1,3-dichloro-2-propyl)phosphate, tributyl citrate, diethyl phthalate, galaxolide, octocrylene, piperonyl butoxide, cis-1,4-dimethylcyclooctane.

# 1. Introduction

## 1.1 Organic micropollutants

Organic micropollutants, also called trace organic contaminants, refers to a diverse and expanding array of natural and anthropogenic substances including industrial chemicals, biocides and pesticides, chemicals used in households, pharmaceuticals and their metabolites excreted by people, and by-products formed during water treatment processes. These organic micropollutants, in the European context of the Water Framework Directive (EU Commission 2000), include compounds considered priority hazardous substances, as well as contaminants of emerging concern (CEC). CECs are new compounds or molecules that were previously unknown or that have just recently appeared in the scientific literature (Stefano et al., 2022). Every year hundreds of new chemicals, including transformation products of existing contaminants, appear in the environment, raising concerns about human exposure and health effects. The necessity to detect and elucidate the structures of these chemicals to assess exposure is indisputable (Paszkievicz et al., 2022).

Organic micropollutants are thus currently ubiquitous in the aquatic environment, including groundwater, surface waters and all diverse types of wastewaters. These implies extra pressure on urban water management and delivering adequate treated water, especially when water reclamation and reuse is needed to alleviate water stress (Biswal & Balasubramanian 2022).

MULTISOURCE proposes to tackle these issues by performing risk assessment of the water quality based on chemical and microbiological monitoring data from the various MULTISOURCE Enhanced Natural Treatment Solutions pilots (ENTS-pilots). Here, chemical data includes organic micropollutants. To do this, the project counts i) with an extended monitoring approach including 61 compounds of interest in wastewater and 31 compounds in road runoff water that are being quantified (WP1), and ii) with this current qualitative work which aimed to identify unknown and new hazardous organic chemicals occurring in the water entering and leaving the ENTS. The ultimate goal, addressed in this report, is to assess if the target monitoring methods should be updated with new compounds of interest.

## 1.2 Non target screening (NTS)

Recent advances in analytical instrumentation have enabled new analytical approaches, which allow us to identify all substances present in a given sample – this is called in the environmental chemistry field a non-target screening approach. These new methods imply that we do not target specific compounds that we look for, demanding pre-determined knowledge on which pollutants can potentially be there. Instead, we can investigate a sample without being biased by “expectations”.

High-resolution mass spectrometers (HRMS) with high mass accuracy and resolution, as well as wide mass ranges, can provide exact masses and resolve peaks with small mass differences, which makes them suitable for the simultaneous detection of thousands of substances. The most used HRMS techniques for the suspect and non-target screening studies in environmental samples include Quadrupole Time of Flight (QToF) and Orbitrap mass spectrometers. These HRMS are either coupled to liquid chromatography (LC) or gas chromatography (GC), allowing the screening of polar and non-polar emerging contaminants, respectively (Hayward et al., 2011; Rostkowski et al., 2019; Thurman et al., 2005). The analytical-qualitative work is usually approached in two workflows: i) suspect screening and ii) non-target analysis. Suspect screening has been said to focus on “known unknowns”, whose compound name and structures are defined and suspect of being present in the sample, while non-target analysis focus on analysing “unknown unknowns” without *a priori* criteria (Paszkievicz et al., 2022).

Traditional target analytical methodologies are designed for the quantification of a small fraction of target substances present in the environment. On one hand, mainly due to the complexity of matrices and the

consequent need for selectivity. On the other hand, due to the availability of analytical standards and the labour-intensive method optimization and validation. For the qualitative work approach, suspect screening aims to confirm the presence of suspected compounds in a sample, typically without a reference standard, but with preliminary information on exact mass and isotope pattern from the molecular formula or the expected adduct(s). Thus, comparing peaks against an existing pre-determined list of compounds of interest, for which MS data is available. In non-target screening, no information is available on the compounds present in the sample and the information about the substances is derived solely from the chromatograms and mass spectra. The structure of a compound that might be present in the sample is suggested, while often leaving the final compound annotation open. Non-target screening can also include exploratory statistical tools of principal component analysis (PCA), differential analysis (DA) and/or Kendrick mass defect plots, all used to fingerprint chemical features of different samples (Gravert et al., 2021). In the present work, the major focus was placed on delivering a systematic and comprehensive suspect screening approach (further explained – section 2.2 to 2.4).

### 1.3 MULTISOURCE ENTS Pilots

Nature-Based Solutions for Water Treatment (NBS<sup>WT</sup>) are green infrastructure components that can be used for managing water, stormwater, and wastewater in urban environments and provide improved water quality and other co-benefits (Oral et al. 2020). One of the MULTISOURCE goals is to deliver new knowledge about ENTS and their ability to remove waterborne contaminants, as well as provide effective risk reduction for chemical and biological hazards.

A total of seven technical pilots are being operated to demonstrate innovative, compact, and effective treatment of a wide range of urban waters (raw wastewater, primary-treated wastewater, combined sewer overflow, greywater, road runoff, and rainwater). The pilots are located in seven different countries (FR, US, BE, IT, ES, NO, DE), representing established solutions, in the sense that their Technology Readiness Levels at the beginning of the project are TRL5-7 and are expected to reach TRL7-9 by the end of the project. All pilots are constructed at a scale for validation and demonstration in relevant and/or operational environments (20 m<sup>2</sup> to 5,500 m<sup>2</sup>). Pilots are being monitored (WP1) with conventional as well as innovative digital tools to establish the dynamic functionality over time and during variations in flow, pollutant loads and climate conditions. Table 1 provides an overview of the pilots, as well as the type of samples provided for this part of the project. For details of each pilot and the respective tailored monitoring plan the reader is directed to the report of MULTISOURCE milestone 1 and respective annexes.

**Table 1** Overview of the ENTS pilots and samples collected for the NTS

Pilot	Country	Water Type	Technology	Inlet/Outlet	Time series	ID	Total number of samples
1	France	Wastewater CSO	Treatment wetland (Rhizo, HA, CSO)	Inlet	No	1-FR-WW-RZ-IN	7
						1-FR-WW-HA-IN	7
						1-FR-CSO-IN	1
2	USA	Wastewater	Treatment wetland	Inlet	No	2-US-WW-IN	3
3	Belgium	Black water	Phytoparking	Inlet/outlet	Yes	3-BE-BW-IN/OUT	8/8
		Grey water				3-BE-GW-IN/OUT	8/8

4	Italy	CSO	Treatment wetland	Inlet/outlet	No	4-IT-CSO-IN/OUT	2/2
5	Spain	Grey water	Green wall	Inlet	No	5-ES-GW-IN	6
6	Norway	Road runoff	Raingarden	Inlet/outlet	No	6-NO-RW-IN/OUT	2/2
7	Germany	Rainwater	Green roof (Carport, Gravel, Intensive, Extensive, Wetland)	Outlet	No	7-DE-RAIN-CP-OUT	1
		Grey water	Green roof	Inlet/Outlet		7-DE-RAIN-GR-OUT	1
						7-DE-RAIN-INT-OUT	1
						7-DE-RAIN-EXT-OUT	1
						7-DE-RAIN-WET-OUT	1
						7-DE-GW-IN/OUT	1/1

## 1.4 Scope and objective

This document reports on the work carried out in MULTISOURCE Task 2.1 - *Non-target screening of unknown and new pollutants and microplastics in pilots*, regarding the suspect screening of organic chemicals. It specifically addresses WP2 - Risk Assessment specific objective to identify unknown and new hazardous organic chemicals in the ENTS pilots.

## 2. Materials and methods

### 2.1 Sample Collection, Transport and Preservation

All samples listed in Table 1 have been collected during the year of 2022. Samples were collected by each pilot operator following the requirements issued by WP1 – ETNS Pilots, described in “Sampling guidelines for micropollutants analysis and microplastic analysis” by Aarhus University and NIVA (2022). In short, water for organic micropollutant analysis was sampled and stored in glass materials and the sample handling have been kept to a minimum. Samples were kept cold (around 5 °C) immediately after collection and frozen at -20 °C until shipment. Transport was done in a thermal box with dry ice or ice gel bricks by express courier services. All samples arrived to Aarhus University from Europe in less than 2 days and from USA in less than 5 days. All samples have reached Aarhus University at < 5 °C and have been immediately frozen at -20 °C until micropollutant analysis. All samples were processed for LC-MS analysis (section 2.1) up to 1 month after collection and for the GC-MS workflow (section 2.2) up to 4 months after collection.

The samples from France contain only inlet, however, the inlet of treatment wetland “HA” represents outlet of treatment wetland “RZ”. The samples from USA contain only inlet because outlet samples were damaged during the transportation. These samples were collected in the end of the seasonal operation of the pilot (April 2022) and could not be retaken. The samples from Spain comprise only inlet because the pilot treating the inlet had not been constructed in 2022. Lower number of samples from Italy and Germany (in comparison to e.g., Belgian pilot) is explained by the dry year and lack of rain events, whereas the Norwegian pilot for most of the 2022 had been under construction.

## 2.2 GC-HRMS workflow

Around 100 mL samples, spiked with recovery mixture, were extracted with 1 mL toluene using magnetic stirring for 15 min, followed by a rest period of 10 min. The supernatants, containing toluene and small amount of water, were transferred to 12 mL vials and then centrifuged at 604 g force for 5 min. Afterwards these extracts were placed in a freezer at -20 °C overnight to freeze the water. Finally, the 12 mL vials were taken out of the freezer and the toluene fraction was immediately poured into a 1 mL vial.

A GC-Orbitrap (Q Exactive, Thermo Fisher) was used to analyze the toluene extracts. A TG-5SILMS (Thermo Fisher, Length: 30 m, I.D: 0.25 mm and film thickness: 0.25 µm) with 5 m safe guide capillary column was used to separate the organic contaminants in the samples. The oven temperature was programmed at 100 °C for 5 min, followed by an increase to 320 °C at 10 °C/min, and then 320 °C held for 5 min. The Orbitrap was operated under the positive electron ionization (EI) mode at 70 eV. The Orbitrap was programmed to analyse a mass range of 60-900 Da in high-resolution mode with mass error of 1 ppm. The temperature of transfer line and ion source was 270 and 280 °C, respectively. A solvent delay of 5 min was used to prevent damage of the filament of the ion source.

The suspect screening of GC-HRMS data was conducted by TraceFinder 4.0 (Thermo Fisher). An in-house suspect library (see section 2.4) for suspect screening on GC was built up with a total of 196 GC-capable chemicals. The mass spectrum obtained from the samples was first deconvoluted. The peaks from the mass spectrum were picked up based on several criteria: mass error < 5 ppm, signal noise ratio (S/N) > 10, TIC intensity > 5000 and ion overlap window > 95%. The peaks were then matched with the in-house library. Identification of the compounds on the suspect list was confirmed with library hit score > 75 and sample/blank ratio > 10. On a second step, suspect screening of GC-HRMS data was conducted by matching NIST and MassBank libraries to identify compounds out of suspect list. The compounds were confirmed by library hit score > 95 and sample/blank ratio > 10.

## 2.3 LC-HRMS workflow

Samples have been analysed in two batches: the batch which reached the AU before August, and before December of 2022. Every sample from each batch has been analysed for four LC/MS combinations: reverse phase chromatography with positive ionisation, reverse phase chromatography with negative ionisation, hydrophilic interaction liquid chromatography (HILIC) with positive ionisation and HILIC chromatography with negative ionisation. Only the data from the reverse phase positive ionisation acquisitions, which also matches the acquisition of the MULTISOURCE target quantification workflows, has been treated and is presented in this report. The suspect screening acquisition of other three modes is kept for a potential retrospective data analysis.

Glass vials with wastewater were centrifuged at 4000 g force for 7 min. to settle particles. 900 µL of each supernatant was transferred into an HPLC autosampler vial, mixed with 100 µL of internal standard solution and analyzed by injecting 10 µL of the mixtures in duplicates into a high-performance liquid chromatography coupled to a 6600 quadrupole high resolution time-of-flight mass spectrometer (UPLC-QTOF) (ABSciex, Framingham, MA, USA). 10 µL samples were injected into the UPLC-QTOF and an Acquity UPLC BEH Shield RP18 column thermostated at 30 °C was used for chromatographic separation. The mobile phases were water (A) and methanol (B), both containing 0.1 % formic acid, mixing total of 300 µg/L in the following gradient elution: 0 min 0% B, 0–9 min 80% B, 9-11 min 100% B, 11–16 min 100% B, 16–16.1 min 0% B, 16.1 min 0% B. The QTOF mass spectrometer was equipped with an electrospray ionization source (ESI) operated in positive ionization mode, with 500 °C heater gas temperature and 5300 V capillary voltage. Information-dependent acquisition (IDA) method was employed to detect samples on the HPLC-QTOF. One IDA cycle contained a TOF MS scan (mass scan range from 100 to 1000 Da, accumulation time 0.25 s) and a Product Ion scan (fragmenting the 10 highest peaks with intensity higher than 100 cps, mass scan range from 25 to 1000 Da, accumulation time of 0.04 s per ion, and collision energy 30 eV with a spread of 15 eV (30 ± 15 eV)).



The acquired data was analyzed by the Sciex OS software (ABSciex, Frammingham, MA, USA). The compounds have been reported if they have not been detected in blank (methanol) samples and have been recorded in duplicate injections in signal to noise ratio higher than 4 and by > 70% library hit score, set by precursor mass tolerance 0.04 Da and fragment mass tolerance 0.4 Da. The maximum acceptable molecular mass error used was 20 ppm, after validation of the workflow against our quality control standards to avoid false negatives. The libraries used include the MULTISOURCE suspect screening list, as well as Sciex libraries: Natural\_Products\_HR-MS/MS\_2.0, Pesticide HR-MS/MS\_1.0, Metabolite HR-MS/MS\_1.0, Antibiotic HR-MS/MS\_1.0, Fluorochemical HR-MS/MS\_2.0, Forensic HR-MS/MS\_2.1 and Mycotoxin HR-MS/MS\_1.0

## 2.4 Data analysis

The MULTISOURCE suspect screening list containing initially 307 potential micropollutants was created based on the methods applied by the Aarhus University, public documents associated to the European Water Framework Directive, recordings of emerging micropollutants in recent peer-reviewed literature and MULTISOURCE internal consultations in 2021.

This list was used to create an in-house library for the GC- and LC-workflows described above. Results from each were then gathered and merged to create a unified results table with detected compounds ([Master Results](#)). The compounds identified by the suspect and non-target screening were classified at different identification confidence levels, according to Schymanski et al. (2014):

*Level 1:* The structure is full confirmed by a reference standard;

*Level 2:* (a) A probable structure is proposed on library spectra hit by matching MS and MS/MS spectra;

(b) A probable structure is proposed by library spectra hit but without clear MS/MS spectra matching

*Level 3:* Top-ranked candidates of structure of the peak are proposed from prediction software in combination with database searches, e.g. ChemSpider or PubChem;

*Level 4:* Only an unequivocal molecular formula can be proposed but no structure information;

*Level 5:* Only exact mass of interest is available.

In reality, due to the high level of filtration in the present data treatment, peaks providing results between Level 5 and 3 are not included in the final results table. The summary result table (Table 2) contains a few selected compounds with Level 2 and 1 identification.

## 3. Results and discussion

In total 3708 features were identified among all the measured samples by GC-Orbitrap. After matching with our suspect list (section 2.4), 16 compounds from the list were found ([Master results](#)). These 16 compounds include four PAHs, five organophosphate flame retardants, two benzothiazoles, two pharmaceuticals and three consumer product additives. These compounds were considered as identified with confidence level 2a. In addition, PAHs were further confirmed by applying a target method, and one more PAH was found by target analysis with identification confidence level 1. Furthermore, after matching with NIST and MassBank libraries, 2936 features were annotated. From this, 50 additional compounds were identified after filtering with library hit score and sample/blank ratio, as well as manual review of mass spectrum. These 50 compounds identified by GC-Orbitrap were assigned an identification confidence level 2b. The categories of these 50 compounds are very diverse, including plasticizers, pesticides, pharmaceuticals, food additives, UV filters, fragrances, metabolites and natural products.

**Table 2** Selected detected compounds by GC- and LC- HRMS

Name	CAS Nr.	Level	Occurrence (n/20)	Group	Category*
Benzo[k]fluoranthene	207-08-9	1	12	TAR	PAHs
Pyrene	129-00-0	1	11	TAR	PAHs
Anthracene	102-12-7	1	10	TAR	PAHs
Caffeine	58-08-2	1	9	TAR	CNS stimulant
N, N-Diethyltoluamide (DEET)	134-62-3	1	9	TAR	Insect repellent
Losartan	114798-26-4	1	7	TAR	Pharmaceutical
Carbamazepine	298-46-4	1	6	TAR	Pharmaceutical
Irbesartan	138402-11-6	1	6	TAR	Pharmaceutical
Phenanthrene	85-01-8	1	6	TAR	PAHs
Fluoranthene	206-44-0	1	5	TAR	PAHs
Benzoylcegonine	519-09-5	1	5	TAR	Metabolite of a drug of abuse
Fexofenadine	83799-24-0	1	5	TAR	Pharmaceutical
Tris(1-chloro-2-propyl) phosphate	13674-84-5	2a	9	SUS	Organophosphate flame retardants
2-(Methylthio)benzothiazole	615-22-5	2a	7	SUS	Benzothiazoles
Benzophenone	119-61-9	2a	6	SUS	UV filters
Triphenyl phosphate	115-86-6	2a	4	SUS	Organophosphate flame retardants
Tris(1,3-dichloro-2-propyl)phosphate	13674-87-8	2a	4	SUS	Organophosphate flame retardant
Tributyl citrate	77-94-1	2b	15	NON	Plasticizer
Diethyl Phthalate	84-66-2	2b	15	NON	Plasticizer
Galaxolide	1222-05-5	2b	13	NON	Fragrance
Strychnine	57-24-9	2a	11	NON	Pesticide
Guanosine	118-00-3	2a	10	NON	Personal care product
Indoxyl	480-93-3	2a	10	NON	Fragrance
Octocrylene	6197-30-4	2b	8	NON	UV filter
Piperonyl butoxide	51-03-6	2b	7	NON	Pesticide
Acetaminophen	103-90-2	2a	5	NON	Pharmaceutical
2'-Deoxyguanosine	961-07-9	2a	5	NON	Personal care product
Naproxen	22204-53-1	2a	5	NON	Pharmaceutical
cis-1,4-Dimethylcyclooctane	13151-99-0	2b	5	NON	Consumer product additive
perfluoropropane sulfonamido propyl dimethyl quaternary amine propanoate	89148-24-3	2b	5	NON	PFAS
Hydroxyethylflurazepam	67263-28-9	2a	4	NON	Pharmaceutical TP
N-Desmethyl-tramadol	75377-45-6	2a	4	NON	Pharmaceutical TP

\* registered use in PubChem database

For the LC-QTOF analysis, depending on the purity of the sample (rainwater contains fewer interfering compounds than black water), up to 4000 features per sample were identified. Applying all criteria listed in section 2.3 of this report and matching the features with the available libraries, which comprised urban water relevant compounds, 119 compounds have been identified, 98 of which have not been included in the MULTISOURCE target list and 96 not in the suspect screening list. Out of these compounds the most frequently occurring among the pilots were pharmaceuticals acetaminophen, indoxyl and fexofenadine; ingredients of personal care products deoxyguanosine and guanosine; plasticizer dibutyl phthalate; pesticide strychnine; detergent lithocholic acid; polyfluorinated substance perfluoropropane sulfonamido propyl dimethyl quaternary amine propanoate and a sweetener L-Sorbose. Also, the recurring pharmaceutical fexofenadine which had been recently included in the MULTISOURCE wastewater target list.

After summarizing and comparing the compounds identified by GC- and HPLC-HRMS, a final list containing 181 identified compounds was generated ([Master results](#)). We found four compounds, androstenedione, caffeine, carbamazepine and DEET, that were identified by both GC-EI- and HPLC-ESI (+)- HRMS. Caffeine, carbamazepine and DEET were also quantified by HPLC-MS/MS (data not shown), showing better detection limits than that by suspect screening on GC-Orbitrap.

The 181 identified compounds were divided into three groups. The compounds on our original target list and identified by target method, classified as group 'TAR'. The compounds on our original suspect list and identified by the suspect were classified as group 'SUS'. The compounds, which are not on our target and suspect list, that identified by matching with other libraries available in our software, were considered as group 'NON'. 27 (TAR) and 10 (SUS) compounds were detected from target and suspect list, respectively. There were 144 compounds identified in the group of 'NON'. Among the 144 compounds, 49 compounds were identified by GC-Orbitrap and 95 compounds were identified by HPLC-QTOF.

In order to prioritize the identified compounds for future inclusion in the target methods, the selected factor to take into account was frequency of occurrence. As shown in Table 1, in total 20 sample types were investigated for this report, including different countries/pilots, treatment technologies and inlet/outlet. The occurrence of the detected compounds was calculated ([Master results](#)), and the detected compounds with higher frequencies were summarized in Table 2. Out of the 181 identified compounds, 83 compounds were found in only one of the samples, while 147 compounds were found up to only 4 times. The most frequent, 34 compounds (occurrence > 4 times) are distributed between TAR, SUS and NON.

## 4. Conclusion

Five compounds in the group of SUS (occurrence  $\geq 4$  times) and 15 compounds in the group of NON (occurrence > 4 times, excluding three lipids and three food additives) are proposed at this stage to be included in the MULTISOURCE target methods:

LC-MS/MS: strychnine, guanosine, indoxyl, acetaminophen, 2'-deoxyguanosine, naproxen, perfluoropropane sulfonamido propyl dimethyl quaternary amine propanoate, hydroxyethylflurazepam and N-Desmethyl-cis-tramadol.

GC-MS: tris(1-chloro-2-propyl) phosphate, 2-(methylthio)benzothiazole, benzophenone, triphenyl phosphate, tris(1,3-dichloro-2-propyl)phosphate, tributyl citrate, diethyl phthalate, galaxolide, octocrylene, piperonyl butoxide, cis-1,4-dimethylcyclooctane.

Collaboration work is ongoing with NIVA to perform a second-tier risk assessment -based prioritization for all 147 identified compounds occurring in more than one sample. Chemical standards can be very costly, thus besides the frequency the objective is also to assess the environmental relevancy before starting the laboratory work to include the new compounds in the target methods. PNECs for all compounds have been mapped by NIVA, while AU team is working on a semi-quantitation approach in order to complete the risk assessment. However, this work is outside of the scope of the present report.

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## ANNEX 1: MULTISOURCE Suspect List

The MULTISOURCE Suspect Screening List was proposed by AU in 2021 to be measured in all pilots. From this extensive list, the compounds marked in the field "Target" are also proposed to be quantified in the Road runoff Water (**RW**) and WasteWater (**WW**), respectively.

Other abbreviations used in the table are **WFD**: The EU Water Framework Directive (which includes "priority substances", substances of emerging concern, as well as compounds inserted in watch lists); **PAHs**: Polycyclic Aromatic Hydrocarbons; **TP**: Transformation Product; **AU**: Aarhus University; (**MUDP/CWP**: internal abbreviations of methods at the AU).

**Table A1.** MULTISOURCE Suspect Screening List

Target	No.	Name	CAS	Reason	Reason 2	Reason 3
-	1	<a href="#">1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin</a>	<a href="#">3268-87-9</a>	WFD priority		
-	2	<a href="#">1,2,3,4,6,7,8,9-Octachlorodibenzofuran</a>	<a href="#">39001-02-0</a>	WFD priority		
-	3	<a href="#">1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin</a>	<a href="#">35822-46-9</a>	WFD priority		
-	4	<a href="#">1,2,3,4,6,7,8-Heptachlorodibenzofuran</a>	<a href="#">67562-39-4</a>	WFD priority		
-	5	<a href="#">1,2,3,4,7,8,9-Heptachlorodibenzofuran</a>	<a href="#">55673-89-7</a>	WFD priority		
-	6	<a href="#">1,2,3,4,7,8-Hexachlorodibenzodioxin</a>	<a href="#">39227-28-6</a>	WFD priority		
-	7	<a href="#">1,2,3,4,7,8-Hexachlorodibenzofuran</a>	<a href="#">70648-26-9</a>	WFD priority		
-	8	<a href="#">1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin</a>	<a href="#">57653-85-7</a>	WFD priority		
-	9	<a href="#">1,2,3,6,7,8-Hexachlorodibenzofuran</a>	<a href="#">57117-44-9</a>	WFD priority		
-	10	<a href="#">1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin</a>	<a href="#">19408-74-3</a>	WFD priority		
-	11	<a href="#">1,2,3,7,8,9-Hexachlorodibenzofuran</a>	<a href="#">72918-21-9</a>	WFD priority		
-	12	<a href="#">1,2,3,7,8-Pentachlorodibenzo-p-dioxin</a>	<a href="#">40321-76-4</a>	WFD priority		
-	13	<a href="#">1,2,3,7,8-Pentachlorodibenzofuran</a>	<a href="#">57117-41-6</a>	WFD priority		
-	14	<a href="#">1,2,5,6,9,10-Hexabromocyclododecane</a>	<a href="#">3194-55-6</a>	WFD priority		
-	15	<a href="#">1,2-Dichloroethane</a>	<a href="#">107-06-2</a>	WFD		
-	16	<a href="#">1,3,5,7,9,11-Hexabromocyclododecane</a>	<a href="#">25637-99-4</a>	WFD priority		
-	17	<a href="#">2,3',4,4',5'-Pentachlorobiphenyl</a>	<a href="#">65510-44-3</a>	WFD priority		
-	18	<a href="#">2,3',4,4',5-Pentachlorobiphenyl</a>	<a href="#">31508-00-6</a>	WFD priority		
-	19	<a href="#">2,3,3',4,4',5'-Hexachlorobiphenyl</a>	<a href="#">52663-72-6</a>	WFD priority		
-	20	<a href="#">2,3,3',4,4',5'-Hexachlorobiphenyl</a>	<a href="#">69782-90-7</a>	WFD priority		
-	21	<a href="#">2,3,3',4,4',5-Hexachlorobiphenyl</a>	<a href="#">38380-08-4</a>	WFD priority		
-	22	<a href="#">2,3,3',4,4'-Pentachlorobiphenyl</a>	<a href="#">32598-14-4</a>	WFD priority		
-	23	<a href="#">2,3,4,4'5-Pentachlorobiphenyl</a>	<a href="#">74472-37-0</a>	WFD priority		
-	24	<a href="#">2,3,4,5,3',4',5'-Heptachlorobiphenyl</a>	<a href="#">39635-31-9</a>	WFD priority		

-	25	<a href="#">2,3,4,6,7,8-Hexachlorodibenzofuran</a>	<a href="#">60851-34-5</a>	WFD priority		
-	26	<a href="#">2,3,4,7,8-Pentachlorodibenzofuran</a>	<a href="#">57117-31-4</a>	WFD priority		
-	27	<a href="#">2,3,7,8-Tetrachlorodibenzo-p-dioxin</a>	<a href="#">1746-01-6</a>	WFD priority		
-	28	<a href="#">2,3,7,8-Tetrachlorodibenzofuran</a>	<a href="#">51207-31-9</a>	WFD priority		
-	29	<a href="#">3,4,3',4'-Tetrachlorobiphenyl</a>	<a href="#">32598-13-3</a>	WFD priority		
-	30	<a href="#">3,4,4',5-Tetrachlorobiphenyl</a>	<a href="#">70362-50-4</a>	WFD priority		
-	31	<a href="#">3,4,5,3',4',5'-Hexachlorobiphenyl</a>	<a href="#">32774-16-6</a>	WFD priority		
-	32	<a href="#">3,4,5,3',4'-Pentachlorobiphenyl</a>	<a href="#">57465-28-8</a>	WFD priority		
-	33	<a href="#">4-(1,1',3,3'-tetramethylbutyl)-phenol</a>	<a href="#">140-66-9</a>	WFD		
-	34	<a href="#">4-Nonylphenol</a>	<a href="#">104-40-5</a>	WFD priority		
-	35	<a href="#">4-Nonylphenol (branched)</a>	<a href="#">84852-15-3</a>	WFD priority		
-	36	<a href="#">Aclonifen</a>	<a href="#">74070-46-5</a>	WFD		
-	37	<a href="#">Alachlor</a>	<a href="#">15972-60-8</a>	WFD		
-	38	<a href="#">alpha-Cypermethrin</a>	<a href="#">67375-30-8</a>	WFD		
<b>RW</b>	39	<a href="#">Anthracene</a>	<a href="#">120-12-7</a>	WFD priority	PAHs AU	
-	40	<a href="#">Atrazine</a>	<a href="#">1912-24-9</a>	WFD		
-	41	<a href="#">Benzene</a>	<a href="#">71-43-2</a>	WFD		
<b>RW</b>	42	<a href="#">Benzo(a)pyrene</a>	<a href="#">50-32-8</a>	WFD priority	PAHs AU	PAHs MUDP
<b>RW</b>	43	<a href="#">Benzo(b)fluoranthene</a>	<a href="#">205-99-2</a>	WFD priority	PAHs AU	PAHs MUDP
<b>RW</b>	44	<a href="#">Benzo(g,h,i)perylene</a>	<a href="#">191-24-2</a>	WFD priority	PAHs AU	
<b>RW</b>	45	<a href="#">Benzo(k)fluoranthene</a>	<a href="#">207-08-9</a>	WFD priority	PAHs AU	PAHs MUDP
-	46	<a href="#">beta-Cypermethrin</a>	<a href="#">65731-84-2</a>	WFD		
-	47	<a href="#">Bifenox</a>	<a href="#">42576-02-3</a>	WFD		
-	48	<a href="#">C10-13-chloroalkanes</a>	85535-84-8	WFD priority		
-	49	<a href="#">Cadmium compounds</a>	-	WFD priority		
-	50	<a href="#">Chlorfenvinphos</a>	<a href="#">470-90-6</a>	WFD		
-	51	<a href="#">Chloroform;Trichloromethane</a>	<a href="#">67-66-3</a>	WFD		
-	52	<a href="#">Chlorpyrifos</a>	<a href="#">2921-88-2</a>	WFD		
<b>RW</b>	53	<a href="#">Cybutryne</a>	<a href="#">28159-98-0</a>	WFD	Pesticides AU	
-	54	<a href="#">Cypermethrin</a>	<a href="#">52315-07-8</a>	WFD		
-	55	<a href="#">zeta-Cypermethrin</a>	<a href="#">52315-07-8</a>	WFD		

-	56	<a href="#">DEHP;Di(2-ethylhexyl)phthalate</a>	<a href="#">117-81-7</a>	WFD priority		
-	57	<a href="#">Derivatives of Perfluorooctane sulfonic acid</a>	-	WFD priority		
-	58	<a href="#">Dichloromethane</a>	<a href="#">75-09-2</a>	WFD		
-	59	<a href="#">Dichlorvos</a>	<a href="#">62-73-7</a>	WFD		
-	60	<a href="#">Dicofol</a>	<a href="#">115-32-2</a>	WFD priority		
-	61	<a href="#">Dioxin-like polychlorinated biphenyls (PCB-DL)</a>	-	WFD priority		
-	62	<a href="#">Dioxins and dioxin-like compounds</a>	-	WFD priority		
<b>RW</b>	63	<a href="#">Diuron</a>	<a href="#">330-54-1</a>	WFD	Pesticides AU	
-	64	<a href="#">Endosulfan</a>	<a href="#">115-29-7</a>	WFD priority		
<b>RW</b>	65	<a href="#">Fluoranthene</a>	<a href="#">206-44-0</a>	WFD	PAHs AU	PAHs MUDP
-	66	<a href="#">Heptabromodiphenyl ethers</a>	<a href="#">68928-80-3</a>	WFD priority		
-	67	<a href="#">Heptachlor</a>	<a href="#">76-44-8</a>	WFD priority		
-	68	<a href="#">Heptachlor epoxide</a>	<a href="#">1024-57-3</a>	WFD priority		
-	69	<a href="#">Hexabromodiphenyl ethers</a>	<a href="#">36483-60-0</a>	WFD priority		
-	70	<a href="#">Hexachlorobenzene</a>	<a href="#">118-74-1</a>	WFD priority		
-	71	<a href="#">Hexachlorobutadiene</a>	<a href="#">87-68-3</a>	WFD priority		
-	72	<a href="#">Hexachlorocyclohexane</a>	<a href="#">608-73-1</a>	WFD priority		
<b>RW</b>	73	<a href="#">Indeno(1,2,3-cd)pyrene</a>	<a href="#">193-39-5</a>	WFD priority	PAHs AU	
<b>WW,R W</b>	74	<a href="#">Isoproturon</a>	<a href="#">34123-59-6</a>	WFD	Pesticides AU	
-	75	<a href="#">Lead compounds</a>	-	WFD		
-	76	<a href="#">Mercury compounds</a>	-	WFD priority		
<b>RW</b>	77	<a href="#">Naphthalene</a>	<a href="#">91-20-3</a>	WFD	PAHs AU	PAHs MUDP
-	78	<a href="#">Nickel compounds</a>	-	WFD		
-	79	<a href="#">Nonylphenols</a>	-	WFD priority		
-	80	<a href="#">Octylphenol</a>	<a href="#">1806-26-4</a>	WFD		
-	81	<a href="#">Octylphenols</a>	-	WFD		
-	82	<a href="#">Pentabromodiphenyl ethers</a>	<a href="#">32534-81-9</a>	WFD priority		
-	83	<a href="#">Pentachlorobenzene</a>	<a href="#">608-93-5</a>	WFD priority		
-	84	<a href="#">Pentachlorophenol</a>	<a href="#">87-86-5</a>	WFD		
-	85	<a href="#">Perfluorooctane sulfonic acid (PFOS)</a>	<a href="#">1763-23-1</a>	WFD priority	PFAS AU	
-	86	<a href="#">Polyaromatic hydrocarbons (PAH)</a>	-	WFD priority		

-	87	<a href="#">Polychlorinated dibenzo-p-dioxins (PCDDs)</a>	-	WFD priority	
-	88	<a href="#">Polychlorinated dibenzofurans (PCDFs)</a>	-	WFD priority	
-	89	<a href="#">Quinoxifen</a>	<a href="#">124495-18-7</a>	WFD priority	
-	90	<a href="#">Simazine</a>	<a href="#">122-34-9</a>	WFD	
<b>RW</b>	91	<a href="#">Terbutryn</a>	<a href="#">886-50-0</a>	WFD	Pesticides AU
-	92	<a href="#">Tetrabromodiphenyl ethers</a>	<a href="#">40088-47-9</a>	WFD priority	
-	93	<a href="#">theta-Cypermethrin</a>	<a href="#">71697-59-1</a>	WFD	
-	94	<a href="#">Tributyltin</a>	<a href="#">688-73-3</a>	WFD priority	
-	95	<a href="#">Tributyltin compounds</a>	-	WFD priority	
-	96	<a href="#">Tributyltin-cation</a>	<a href="#">36643-28-4</a>	WFD priority	
-	97	<a href="#">Trichlorobenzenes</a>	<a href="#">12002-48-1</a>	WFD	
-	98	<a href="#">Trifluralin</a>	<a href="#">1582-09-8</a>	WFD priority	
-	99	<a href="#">α-Hexabromocyclododecane</a>	<a href="#">134237-50-6</a>	WFD priority	
-	100	<a href="#">β-Hexabromocyclododecane</a>	<a href="#">134237-51-7</a>	WFD priority	
-	101	<a href="#">γ-Hexabromocyclododecane</a>	<a href="#">134237-52-8</a>	WFD priority	
-	102	Metaflumizone	<a href="#">139968-49-3</a>	WFD watch	
<b>WW</b>	103	Amoxicillin	<a href="#">26787-78-0</a>	WFD watch	CWP2
<b>WW</b>	104	Ciprofloxacin	<a href="#">85721-33-1</a>	WFD watch	CWP1
<b>WW</b>	105	Sulfamethoxazole	<a href="#">723-46-6</a>	WFD watch	CWP1
-	106	Trimethoprim	<a href="#">738-70-5</a>	WFD watch	
<b>WW</b>	107	Venlafaxine	<a href="#">93413-69-5</a>	WFD watch	CWP1
-	108	O-desmethylvenlafaxine	<a href="#">93413-62-8</a>	WFD watch	
-	109	Clotrimazole	<a href="#">23593-75-1</a>	WFD watch	
-	110	Fluconazole	<a href="#">86386-73-4</a>	WFD watch	
-	111	Imazalil	<a href="#">35554-44-0</a>	WFD watch	
-	112	Ipconazole	<a href="#">125225-28-7</a>	WFD watch	
-	113	Metconazole	<a href="#">125116-23-6</a>	WFD watch	
<b>WW</b>	114	Miconazole	<a href="#">22916-47-8</a>	WFD watch	CWP2
-	115	Penconazole	<a href="#">66246-88-6</a>	WFD watch	
-	116	Prochloraz	<a href="#">67747-09-5</a>	WFD watch	
<b>RW</b>	117	Tebuconazole	<a href="#">107534-96-3</a>	WFD watch	Pesticides AU
-	118	Tetraconazole	<a href="#">112281-77-3</a>	WFD watch	
-	119	Dimoxystrobin	<a href="#">149961-52-4</a>	WFD watch	



-	120	Famoxadone	<a href="#">131807-57-3</a>	WFD watch		
WW	121	Atenolol	<a href="#">29122-68-7</a>	CWP1		
WW	122	Sotalol	<a href="#">3930-20-9</a>	CWP1		
WW	123	Diatrizoic acid	<a href="#">117-96-4</a>	CWP1		
WW	124	Iohexol	<a href="#">66108-95-0</a>	CWP1		
WW	125	Iomeprol	<a href="#">78649-41-9</a>	CWP1		
WW	126	Iopamidol	<a href="#">60166-93-0</a>	CWP1		
WW	127	Iopromide	<a href="#">73334-07-3</a>	CWP1		
WW	128	Gabepentin	<a href="#">60142-96-3</a>	CWP1		
WW	129	Sulfadiazine	<a href="#">68-35-9</a>	CWP1		
WW	130	Trimethoprim	<a href="#">738-70-5</a>	CWP1		
WW	131	Sulfamethizole	<a href="#">144-82-1</a>	CWP1		
WW	132	Metoprolol	<a href="#">37350-58-6</a>	CWP1		
WW	133	Tramadol	<a href="#">27203-92-5</a>	CWP1		
WW	134	Venlafaxine	<a href="#">93413-69-5</a>	CWP1		
WW	135	Clindamycin	<a href="#">18323-44-9</a>	CWP1		
WW	136	Azithromycin	<a href="#">83905-01-5</a>	CWP1		
WW	137	Phenazone	<a href="#">60-80-0</a>	CWP1		
WW	138	Benzotriazole	<a href="#">29385-43-1</a>	CWP1		
WW	139	Propranolol	<a href="#">525-66-6</a>	CWP1		
WW	140	Citalopram	<a href="#">59729-33-8</a>	CWP1		
WW	141	Erythromycin	<a href="#">114-07-8</a>	CWP1		
WW	142	Clarithomycin	<a href="#">81103-11-9</a>	CWP1		
WW	143	Carbamazepine	<a href="#">298-46-4</a>	CWP1		
WW	144	Eprosartan	<a href="#">133040-01-4</a>	CWP1		
WW	145	Olmesartan	<a href="#">144689-63-4</a>	CWP1		
WW	146	Ibuprofen	<a href="#">15687-27-1</a>	CWP1		
WW	147	Diclofenac	<a href="#">15307-86-5</a>	CWP1		
WW	148	Mycophenolic acid	<a href="#">24280-93-1</a>	CWP1		
WW	149	Valsartan	<a href="#">137862-53-4</a>	CWP1		
WW	150	Irbesartan	<a href="#">138402-11-6</a>	CWP1		
WW	151	Losartan	<a href="#">114798-26-4</a>	CWP1		
WW	152	Candesartan	<a href="#">139481-59-7</a>	CWP1		

WW	153	Roxithromycin	<a href="#">80214-83-1</a>	CWP1		
WW	154	Oxazepam	<a href="#">604-75-1</a>	CWP1		
WW	155	Ampicillin	<a href="#">69-53-4</a>	CWP2		
WW	156	Bicalutamide	<a href="#">90357-06-5</a>	CWP2		
WW	157	Ceftazidime	<a href="#">72558-82-8</a>	CWP2		
WW	158	Codeine	<a href="#">76-57-3</a>	CWP2		
WW	159	Estrone	<a href="#">53-16-7</a>	CWP2		
WW	160	Furosemide	<a href="#">54-31-9</a>	CWP2		
WW	161	Gemfibrozil	<a href="#">25812-30-0</a>	CWP2		
WW	162	Lidocaine	<a href="#">137-58-6</a>	CWP2		
WW	163	Mefenamic acid	<a href="#">61-68-7</a>	CWP2		
WW	164	Propyphenazone	<a href="#">479-92-5</a>	CWP2		
WW	165	Ranitidine	<a href="#">66357-35-5</a>	CWP2		
WW	166	Rosuvastatin	<a href="#">287714-41-4</a>	CWP2		
WW	167	Sertraline	<a href="#">79617-96-2</a>	CWP2		
WW	168	Simvastatin	<a href="#">79902-63-9</a>	CWP2		
WW	169	Sulfapyridine	<a href="#">144-83-2</a>	CWP2		
WW	170	Azithromycin' - Azithromycin N-oxides	-	Pharma TP AU		
WW	171	Clarithromycin' - Clarithromycin N-oxides	-	Pharma TP AU		
WW	172	Erythromycin' - Erythromycin N-oxides	-	Pharma TP AU		
WW	173	Sulfadiazine' - Ac-Sulfadiazine	-	Pharma TP AU		
WW	174	Sulfamethoxazole' - Ac-Sulfamethoxazole	-	Pharma TP AU		
WW	175	Sulfamethoxazole' - AMiosX	-	Pharma TP AU		
WW	176	Metoprolol' - Alpha-hydroxymetoprolol	-	Pharma TP AU		
WW	177	Metoprolol' - Metoprolol acid	-	Pharma TP AU		
WW	178	Metoprolol' - O-demethylmetoprolol	-	Pharma TP AU		
WW	179	Carbamazepine' - BaQD 1-(2-benzoic acid)-(1H,3H)-quinazoline-2,4-dione	-	Pharma TP AU		
WW	180	Carbamazepine' - CBZ 10,11 epoxides CBZ-EPX	-	Pharma TP AU		
WW	181	Carbamazepine' - rac trans 10,11 (dihydro, dihydroxy) CBZ-RTN	-	Pharma TP AU		
WW	182	Diclofenac' - DCF 2,5 quinone imine	-	Pharma TP AU		
WW	183	Diclofenac' - DCF amide	-	Pharma TP AU		
WW	184	Diclofenac' - DCF benzoic acid	-	Pharma TP AU		

<b>WW</b>	185	Diclofenac' - 1-(2,6-dichlorophenyl)indolin-2,3-dione DCPID	-	Pharma TP AU		
<b>WW</b>	186	Diclofenac' - 2,6-dichlorodiphenylamine	-	Pharma TP AU		
<b>WW</b>	187	Tramadol' - N-Desmethyl tramadol	-	Pharma TP AU		
<b>WW</b>	188	Tramadol' - Tramadol N-oxide	-	Pharma TP AU		
<b>WW</b>	189	Venlafaxin' - Venlafaxin N-oxide	-	Pharma TP AU		
<b>RW</b>	190	Propiconazole	<a href="#">60207-90-1</a>	Pesticides AU		
<b>WW,R W</b>	191	Carbendazim	<a href="#">10605-21-7</a>	Pesticides AU		
<b>RW</b>	192	Pirimicarb	<a href="#">23103-98-2</a>	Pesticides AU		
<b>WW,R W</b>	193	Azoxystrobin	<a href="#">131860-33-8</a>	Pesticides AU		
<b>RW</b>	194	Pyraclostrobin	<a href="#">175013-18-0</a>	Pesticides AU		
<b>RW</b>	195	Diflufenican	<a href="#">83164-33-4</a>	Pesticides AU		
<b>RW</b>	196	Diazinon	<a href="#">333-41-5</a>	Pesticides AU		
<b>RW</b>	197	Mecoprop	<a href="#">7085-19-0</a>	Pesticides AU		
<b>WW,R W</b>	198	Thiacloprid	<a href="#">111988-49-9</a>	Pesticides		
<b>RW</b>	199	Dimethoate	<a href="#">60-51-5</a>	Pesticides		
<b>RW</b>	200	Imidacloprid	<a href="#">138261-41-3</a>	Pesticides		
<b>WW,R W</b>	201	Benzalkonium chloride (-C <sub>n</sub> H <sub>2n+1</sub> ) n=12	-	Surfactants AU		
<b>WW,R W</b>	202	Benzalkonium chloride (-C <sub>n</sub> H <sub>2n+1</sub> ) n=14	-	Surfactants AU		
<b>WW,R W</b>	203	Benzalkonium chloride (-C <sub>n</sub> H <sub>2n+1</sub> ) n=16	-	Surfactants AU		
<b>RW</b>	204	Diflufenican' - AE-B	-	Pesticide TP AU		
<b>RW</b>	205	Diflufenican' - AE-O	-	Pesticide TP AU		
<b>RW</b>	206	Glyphosate' - Dichlorobenzamide (BAM)	-	Pesticide TP AU		
-	207	PFPeA	<a href="#">2706-90-3</a>	PFAS AU		
-	208	PFHxA	<a href="#">307-24-4</a>	PFAS AU		
-	209	PFHpA	<a href="#">375-85-9</a>	PFAS AU		
-	210	PFHxS	<a href="#">355-46-4</a>	PFAS AU		
-	211	PFBS	<a href="#">375-73-5</a>	PFAS AU		
-	212	PFOA	<a href="#">335-67-1</a>	PFAS AU		
-	213	PFHpS	<a href="#">21934-50-9</a>	PFAS AU		

-	214	PFNA	<a href="#">375-95-1</a>	PFAS AU		
-	215	PFUnA	<a href="#">2058-94-8</a>	PFAS AU		
-	216	PFDoA	<a href="#">307-55-1</a>	PFAS AU		
-	217	PFDS	<a href="#">335-77-3</a>	PFAS AU		
-	218	PFTra	<a href="#">72629-94-8</a>	PFAS AU		
-	219	PFTeA	<a href="#">376-06-7</a>	PFAS AU		
<b>RW</b>	220	Acenaphthylene	<a href="#">208-96-8</a>	PAHs AU		
<b>RW</b>	221	Acenaphthene	<a href="#">83-32-9</a>	PAHs AU		
<b>RW</b>	222	Fluorene	<a href="#">86-73-7</a>	PAHs AU		
<b>RW</b>	223	Dibenzothiophene	<a href="#">132-65-0</a>	PAHs AU		
<b>RW</b>	224	Phenanthrene	<a href="#">85-01-8</a>	PAHs AU	PAHs MUDP	
<b>RW</b>	225	Pyrene	<a href="#">129-00-0</a>	PAHs AU	PAHs MUDP	
<b>RW</b>	226	Benz(a)anthracene	<a href="#">56-55-3</a>	PAHs AU		
<b>RW</b>	227	Chrysene	<a href="#">218-01-9</a>	PAHs AU		
<b>RW</b>	228	Benz(e)pyrene	<a href="#">192-97-2</a>	PAHs AU		
<b>RW</b>	229	Perylene	<a href="#">198-55-0</a>	PAHs AU		
<b>RW</b>	230	Dibenz(a,h)anthracene	<a href="#">53-70-3</a>	PAHs AU		
<b>RW</b>	231	1-methylpyrene	<a href="#">2381-21-7</a>	PAHs AU		
<b>RW</b>	232	Benzo(a)fluorene	<a href="#">238-84-6</a>	PAHs AU		
<b>RW</b>	233	C1-Naphthalenes	-	Alkyl PAHs AU		
<b>RW</b>	234	C2-Naphthalenes	-	Alkyl PAHs AU		
<b>RW</b>	235	C3-Naphthalenes	-	Alkyl PAHs AU		
<b>RW</b>	236	C1-Phenanthrenes	-	Alkyl PAHs AU		
<b>RW</b>	237	C2-Phenanthrenes	-	Alkyl PAHs AU		
<b>RW</b>	238	C3-Phenanthrenes	-	Alkyl PAHs AU		
<b>RW</b>	239	C1-Dibenzothiophenes	-	Alkyl PAHs AU		
-	240	C4-Naphthalenes	-	Alkyl PAHs - other		
-	241	C4-Phenanthrenes	-	Alkyl PAHs - other		
-	242	C1-Fluorenes	-	Alkyl PAHs - other		
-	243	C2-Fluorenes	-	Alkyl PAHs - other		

-	244	C3-Fluorenes	-	Alkyl PAHs - other		
-	245	C1-Anthracenes	-	Alkyl PAHs - other		
-	246	C2-Anthracenes	-	Alkyl PAHs - other		
-	247	C3-Anthracenes	-	Alkyl PAHs - other		
-	248	C4-Anthracenes	-	Alkyl PAHs - other		
-	249	C1-Chrysenes	-	Alkyl PAHs - other		
-	250	C2-Chrysenes	-	Alkyl PAHs - other		
-	251	C3-Chrysenes	-	Alkyl PAHs - other		
-	252	C1-Pyrenes	-	Alkyl PAHs - other		
-	253	C2-Pyrenes	-	Alkyl PAHs - other		
-	254	C1-Fluoranthenes	-	Alkyl PAHs - other		
-	255	C2-Fluoranthenes	-	Alkyl PAHs - other		
-	256	Methyl sulfate	<a href="#">512-42-5</a>	Schulze freq. PMOC		
-	257	Sodium Acryloyldimethyltaurate	<a href="#">5165-97-9</a>	Schulze freq. PMOC		
-	258	Benzyltrimethylammonium chloride	<a href="#">56-93-9</a>	Schulze freq. PMOC		
-	259	Trifluoromethanesulfonic acid	<a href="#">1493-13-6</a>	Schulze freq. PMOC		
-	260	Acetoguanamine	<a href="#">542-02-9</a>	Schulze freq. PMOC		
-	261	Dimethylbenzylamine	<a href="#">103-83-3</a>	Schulze freq. PMOC		
-	262	Ditolyguanidine	<a href="#">97-39-2</a>	Schulze freq. PMOC		
-	263	Amantadine	<a href="#">768-94-5</a>	Schulze freq. PMOC		
-	264	Cyanoguanidine	<a href="#">461-58-5</a>	Schulze freq. PMOC		

-	265	p-Toluenesulfonic acid	<a href="#">104-15-4</a>	Schulze freq. PMOC		
-	266	Sodium 3,4-dimethylbenzenesulfonate	<a href="#">1300-72-7</a>	Schulze freq. PMOC		
-	267	Dimethylbenzenesulfonic acid	<a href="#">25321-41-9</a>	Schulze freq. PMOC		
-	268	Toluenesulfonamide	<a href="#">70-55-3</a>	Schulze freq. PMOC		
-	269	1,3-Diphenylguanidine	<a href="#">102-06-7</a>	Schulze freq. PMOC		
-	270	Acesulfame potassium	<a href="#">55589-62-3</a>	Schulze freq. PMOC		
-	271	Cyanuric acid	<a href="#">108-80-5</a>	Schulze freq. PMOC		
-	272	Metanilate	<a href="#">121-47-1</a>	Schulze freq. PMOC		
-	273	Sulfanilic acid	<a href="#">121-57-3</a>	Schulze freq. PMOC		
-	274	Melamine	<a href="#">108-78-1</a>	Schulze freq. PMOC		
-	275	Naphthalenesulfonic acid	<a href="#">85-47-2</a>	Schulze freq. PMOC		
-	276	Caprolactam	<a href="#">105-60-2</a>	Schulze freq. PMOC		
-	277	Ametryn	<a href="#">834-12-8</a>	Schulze freq. PMOC		
<b>RW</b>	278	Tris(2-chloroisopropyl) phosphate (TCPP)	<a href="#">13674-84-5</a>	Organophosphorus		
<b>RW</b>	279	Tris(2-chloroethyl) phosphate (TCEP)	<a href="#">115-96-8</a>	Organophosphorus		
<b>RW</b>	280	Tri-n-butyl phosphate (TBP)	<a href="#">126-73-8</a>	Organophosphorus		
<b>RW</b>	281	Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	<a href="#">13674-87-8</a>	Organophosphorus		
-	282	Tricresyl phosphate (TCrP)	<a href="#">1330-78-5</a>	Organophosphorus		
<b>RW</b>	283	Triphenyl phosphate (TPhP)	<a href="#">115-86-6</a>	Organophosphorus		
<b>RW</b>	284	Tri-isobutyl phosphate (TiBP)	<a href="#">126-71-6</a>	Organophosphorus		
-	285	Tri-o-cresyl phosphate (ToCrP)	<a href="#">78-30-8</a>	Organophosphorus		

<b>RW</b>	286	Tris(2-butoxyethyl)phosphate (TBEP)	<a href="#">78-51-3</a>	Organophosphorus		
-	287	2-ethylhexyl diphenyl phosphate (EHDPP)	<a href="#">1241-94-7</a>	Organophosphorus		
-	288	Dibutyl phenyl phosphate (DBPhP)	<a href="#">2528-36-1</a>	Organophosphorus		
-	289	Diphenyl butyl phosphate (DPhBP)	<a href="#">2752-95-6</a>	Organophosphorus		
-	290	Tri(2-ethylhexyl)phosphate (TEHP)	<a href="#">78-42-2</a>	Organophosphorus		
<b>RW</b>	291	Hydroxybenzothiazole (OHBT)	<a href="#">934-34-9</a>	Benzothiazoles		
<b>RW</b>	292	Mercaptobenzothiazole (MBT)	<a href="#">149-30-4</a>	Benzothiazoles		
<b>RW</b>	293	Aminobenzothiazole (ABT)	<a href="#">136-95-8</a>	Benzothiazoles		
<b>RW</b>	294	Benzothiazole (BT)	<a href="#">95-16-9</a>	Benzothiazoles		
<b>RW</b>	295	Methylthiobenzothiazole (MTBT)	<a href="#">615-22-5</a>	Benzothiazoles		
<b>WW</b>	296	Caffeine	<a href="#">58-08-2</a>	Other		
<b>WW</b>	297	Benzoylcegonine	<a href="#">519-09-5</a>	Other		
<b>WW</b>	298	THC-COOH	<a href="#">56354-06-4</a>	Other		
<b>WW</b>	299	Amphetamine	<a href="#">300-62-9</a>	Other		
<b>WW</b>	300	Methamphetamine	<a href="#">537-46-2</a>	Other		
<b>WW</b>	301	MDMA	<a href="#">64057-70-1</a>	Other		
<b>WW</b>	302	Benzophenone	<a href="#">119-61-9</a>	Other		
<b>WW</b>	303	Diethyltoluamide (DEET)	<a href="#">134-62-3</a>	Other		
<b>RW</b>	304	Oxalic acid p-phenylenediamine (6PPD)	<a href="#">793-24-8</a>	Other		
<b>RW</b>	305	6PPD-Quinone	-	Other		
<b>WW,R W</b>	306	Didecyldimethylammonium chloride (DDAC)	<a href="#">7173-51-5</a>	Other		
<b>WW,R W</b>	307	Triethylene Glycol Diacetate (TDAC)	<a href="#">111-21-7</a>	Other		

The overall goal of MULTISOURCE is to, together with local, national, and international stakeholders, demonstrate a variety of about Enhanced Natural Treatment Solutions (ENTS) treating a wide range of urban waters and to develop innovative tools, methods, and business models that support citywide planning and long-term operations and maintenance of nature-based solutions for water treatment, storage, and reuse in urban areas worldwide. The project includes seven pilots treating a wide range of urban waters. Two individual municipalities (Girona, Spain; Oslo, Norway), two metropolitan municipalities (Lyon, France; Milan, Italy), and international partners in Brazil, Vietnam, and the USA will contribute to each of the main project activities: ENTS pilots, risk assessment, business models, technology selection, and the MULTISOURCE Planning Platform. The use of urban archetypes in the Planning Platform will enable users to quickly classify regions (in both developed or developing countries) suitable for the application of nature-based solutions for water treatment (NBSWT) and compare scenarios both with and without NBSWT.



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