

Highly Sensitive Determination of Contaminants in Surface Water in the Context of the EU Water Framework Directive using Stir Bar Sorptive Extraction (SBSE) and GC-MS/MS

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KEYWORDS

EU water framework directive (2013/39/EU), stir bar sorptive extraction (SBSE), PDMS Twister, persistent organic pollutant (POP), PAH, PCB, PBDE, organochlorine pesticide (OCP), GC-MS/MS

ABSTRACT

In the work presented here, highly sensitive determination of around 100 contaminants in surface water in the concentration range from low double-digit to low triple-digit pg/L was performed. Priority compounds from the EU water framework directive (EU-WFD) as well as substances from other legislation were included. A sequential stir bar sorptive extraction (SBSE) approach employing the GERSTEL Twister was used for analyte enrichment from 100 mL water samples. The Twister was thermally desorbed, compounds were separated via GC and detected by tandem mass spectrometry (MS/MS) utilizing an Agilent 7010 MS.

The analysis method was comprehensively validated and requirements of the EU-WFD for inland surface water were fulfilled. Repeat analyses of water samples spiked at concentrations close to the Limits of Quantification (LOQ) of the respective analytes demonstrated relative standard deviations between 1 and 15 % with an average of 6.9 %. Trueness was mainly between 90 and 110 %. The correct quantitation of particle-adsorbed compounds like PAHs was examined and confirmed

using certified reference sediment.

Cypermethrin, heptachlor and heptachlorepoide were the only compounds for which the required LOQs could not be reached. To date there is no technique known to the authors that reaches the required LOQs of 0.06 pg/L for heptachlor and heptachlorepoide. The developed analysis method was successfully applied to real world water samples.

INTRODUCTION

In 2000 the European Community issued a directive “to establish a framework for the protection of inland surface waters, transitional waters, coastal waters and groundwater”. This was amended and modified by further directives in 2008 and 2013 [1-3]. Goals are the reduction of surface and ground water pollution as well as to “protect and enhance the status of aquatic ecosystems” and “the protection of territorial and marine waters”. A continuous improvement of water quality shall be pursued to maintain “sufficient supply of good quality surface water and groundwater as needed for sustainable, balanced and equitable water use”. In order to document the present state and to verify the achievements every EU member country is obliged amongst others to test for the “chemical status” of the surface water in each river basin district. The meaning of “chemical status” is substantiated with a list of so called “priority substances” which need to be monitored regularly. Maximum contaminant concentrations

derived from toxicological considerations and aimed at implementation for every EU surface water in the long-run are defined as so called “environmental quality standards” (EQS). Annual average (AA-EQS) and maximum allowable concentrations (MAC-EQS) were established distinguishing between “inland surface waters” like rivers and lakes and “other surface waters” like coastal waters.

Analysis methods employed in the context of EU-WFD need to fulfill certain performance criteria [4]: “Member States shall ensure that the minimum performance criteria for all methods of analysis applied are based on an uncertainty of measurement of 50 % or below ($k = 2$) estimated at the level of relevant environmental quality standards and a limit of quantification equal or below a value of 30 % of the relevant environmental quality standards”. „Where those criteria are not met for any matrix, Member States shall ensure that monitoring is carried out using best available techniques not entailing excessive costs”.

Required LOQs for inland surface water resulting from these specifications, calculated from AA-EQS are challenging for the majority of priority compounds: naphthalene 600 ng/L, chlorpyrifos-ethyl 9 ng/L, p,p'-DDT 3 ng/L, endosulfan 1.5 ng/L, dichlorvos 0.18 ng/L, benzo[a]pyrene 0.051 ng/L, cypermethrin 0.024 ng/L and heptachlor and heptachlorepoxyde 0,00006 ng/L. “The water EQS [...] are expressed as total concentrations in the whole water sample”, meaning that particle-adsorbed analytes must be quantified correctly as well.

Relevant analytes for the method described here were derived from the aforementioned EU-WFD, the Commission Implementing Decision (EU) 2015/495 (“watch list”) [5] and the German Oberflächengewässerverordnung (OGewV, version July 2011) [6]. Only those compounds were included, which could be extracted by polydimethylsiloxane (PDMS) Twisters and separated via gas chromatography. Polar substances of the EU-WFD need to be analyzed by LC-MS/MS, e.g. isoproturon and diuron, volatile compounds like dichloromethane by headspace-GC/MS and metal ions like lead and mercury by inductively coupled plasma mass spectrometry (ICP-MS) or atomic absorption spectroscopy (AAS). The final list contained mainly persistent organic pollutants (POPs) like organochlorine pesticides, PAHs, PCBs and PBDEs as well as other pesticides and industrial pollutants. For analyte enrichment we employed stir bar sorptive extraction (SBSE) using the GERSTEL Twister®. It is a glass-encased magnetic stir bar coated with an

extraction phase of polydimethylsiloxane (PDMS) or ethyleneglycol-polydimethylsiloxane (EG-silicone). While stirring the sample analytes partition between the extractant phase, in this case PDMS, and the liquid sample phase just as in liquid-liquid extraction. Subsequently Twisters are thermally desorbed in the GERSTEL Thermal Desorption Unit (TDU) and analytes are refocused in the Cooled Injection System (CIS) followed by transfer to the GC column and triple quadrupole MS detection in multi reaction monitoring (MRM) mode. Using this setup, all extracted analytes are completely transferred onto the GC-MS/MS making this technique highly sensitive.



Figure 1. Twister PDMS stir bar, 1 cm length, 1 mm phase thickness.

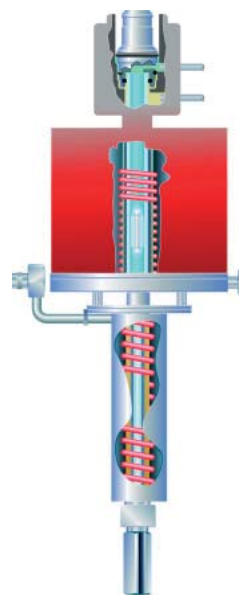


Figure 2. Schematic drawing of the Thermal Desorption Unit (TDU) and the Cooled Injection System (CIS) used for Twister desorption and analyte transfer to the GC.

In order to access a wide variety of compounds and to ensure the extraction of particle-adsorbed compounds, the technique of sequential SBSE developed by Ochiai et. al. [7] was utilized. A single sample aliquot is extracted sequentially by two Twisters under different conditions, for example, with or without salt or solvent addition. Subsequently, both Twisters are desorbed simultaneously resulting in a single chromatogram covering an extended range of analytes.

The aim of our method development was to achieve the determination of around 100 analytes by SBSE-TDU-GC-MS/MS in a single analytical run. The required LOQs for compounds listed in the EU-WFD should be reached while the sample preparation method should be as simple and straightforward as possible. Finally the extraction and correct quantification of particle-adsorbed compounds should be ensured as required by the EU-WFD.

EXPERIMENTAL

Materials and Solvents. For sample extraction 1 cm / 1 mm (length / phase thickness) PDMS Twisters were used (GERSTEL p/n 011333-001-00). The Twisters were conditioned at 280°C under a nitrogen flow overnight using a GERSTEL® Tube Conditioner (TC 2) and stored in the original storage vial until use. Samples were filled into individual 100 mL vials (GERSTEL 093640-062-00), a Twister was added to each vial before closing it with a crimp cap (GERSTEL 011912-002-00). A heated stirring plate was utilized for Twister extraction (GERSTEL 049000-000-NS), along with a dedicated twister removal tool (GERSTEL 013820-001-00) and drying device (GERSTEL 049000-200-00). Organic modifier for the second extraction step was added by a multi dispenser (GERSTEL 049000-100-00) equipped with 50 mL pipette tips (GERSTEL 049000-101-00).

In order to reduce background contamination all glassware was heated at 300°C in a laboratory oven overnight prior use. In the same manner pipette tips were heated at 120°C.

All solvents used were of analytical grade, purchased from different suppliers, including Merck, LGC Standards, Alfa Aesar and Carl Roth.

Preparation of samples and calibration standards. For calibration, one multi-analyte standard in acetone was prepared from certified reference standards and solutions made up from individual neat compounds. Concentrations were adapted to the respective LOQ of each analyte. Three working solutions were diluted from this stock solution to be used for spiking calibration samples. A multi-component internal standard solution was prepared from deuterated or ¹³C analyte analogues in acetone.

Calibration was run over the complete analysis method. To avoid external contamination a 100 g aliquot of pure water was weighed in directly from the primary bottle without using a pipette or similar

device. Subsequently, different amounts of working solution and 30 µL of the internal standard solution were added. Background analyte peaks resulting from the water matrix and the laboratory surrounding should be small compared to the lowest calibration level. Additionally the water used for calibration should be as similar as possible to the water of the real samples. Therefore very clean groundwater, tap water or mineral water were found to be suitable for calibration whereas groundwater gave the best results regarding trueness of analysis values. Samples to be analyzed should have a pH between 5.5 and 7. If necessary the pH value can be adjusted by addition of 0.1 M hydrochloric acid or 0.1 M potassium hydroxide solution. Again 100 g aliquots were weighed in and 30 µL of internal standard solution added before extraction.

A 1 cm / 1 mm PDMS Twister was added to the vial, which was closed with a crimp cap and placed on a Twister stirring plate for extraction at 1000 rpm for 5 h. After that the Twister was briefly rinsed in HPLC water, transferred to a clean desorption tube and dried in a stream of nitrogen for around 10 s since it was found that, in this case, the standard drying procedure employing a lint free tissue was prone to contaminate the Twister. Desorption tubes were stored contamination free on the TDU rack of the MultiPurpose Sampler (MPS). To perform the second step in the sequential SBSE method, a 15 mL volume of an organic modifier was added to each sample vial for subsequent extraction with a second PDMS Twister at 1000 rpm and elevated temperature over a 17 h period. After rinsing in HPLC water the second Twister was combined with the Twister from the first extraction in the same desorption tube and dried as previously mentioned. Twisters placed in TDU tubes were stored in sealed TDU racks on the MPS until they underwent automated thermal desorption.

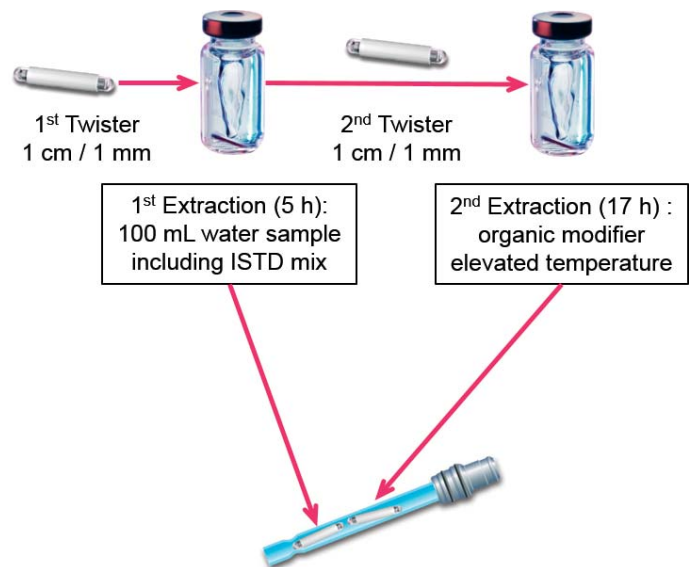
Instrumentation. Analyses were performed using a 7890 GC coupled to a 7010 triple quadrupole MS (both Agilent Technologies), a Thermal Desorption Unit (TDU 2), Cooled Injection System (CIS 4) and MultiPurpose Sampler (MPS Robotic) (all GERSTEL). The MPS automatically delivered Twisters loaded in desorption tubes from the storage rack to the TDU. During thermal desorption, analytes were refocused in the CIS on a Restek Topaz deactivated liner filled with glass wool (GERSTEL 019867-005-00). An HP-5ms Ultra Inert 30 m, d_i=0.25 mm, d_f=0.25 µm from Agilent was utilized for compound separation. Retention times

were locked with chlorpyrifos-methyl (at 18.111 min). Helium was used as carrier gas and quenching gas in the MS collision cell while nitrogen was the collision gas used.



Figure 3. Analysis system used for this application consisting of a GERSTEL® MultiPurpose Sampler (MPS Robotic), a Thermal Desorption Unit (TDU 2), a Cooled Injection System (CIS 4) and an Agilent® Technologies 7890 GC configured with a 7010 triple quadrupole MS.

GC	Agilent 7890B
Column	HP-5ms Ultra Inert (Agilent), 30 m x 0.25 mm x 0.25 µm
Mode	constant flow, 1.0 mL/min (1.5 mL for 3 min, post run)
RTL	chlorpyrifosmethyl @ 18.111 min
Temperature	60°C (1 min), at 40°C/min to 120°C, at 5°C/min to 310°C (post run 325°C)
MS/MS	Agilent 7010
Ionization	Electron impact (EI) at 70 eV (110 eV for cypermethrin and benzo[a]pyrene)
Mode	MRM (see table 1)
Source	300°C
Quadrupole	150°C
Collision gas	N ₂ , 1.5 mL/min
Quenching gas	He, 4 mL/min
Transferline	300°C



Analysis conditions

Thermal Desorption	TDU (GERSTEL)
Tube Type	empty (Twister)
Pneumatics Mode	solvent venting / dry purge (2 min)
Sample Mode	sample remove
Temperature	90°C, at 80°C/min to 300°C (6 min)
Transferzone Temperature	350°C
PTV inlet	CIS 4 (GERSTEL)
Liquid Nitrogen Cooling	
Liner Type	deactivated glass wool
Carrier Gas	Helium
Pneumatics Mode	solvent venting
Vent Flow	80 mL/min
Vent Pressure	57 kPa until 0.1 min
Splitflow	200 mL/min @ 3.01 min (100 mL/min @ 13 min)
Temperature	-40°C, at 12°C/sec to 300°C (5 min), at 12°C/sec to 280°C (37 minutes)

Figure 4. Sequential SBSE extraction workflow employed for analysis of surface water samples.

RESULTS AND DISCUSSION

A thorough method development was essential in order to meet all challenges posed by this application. Many parameters were evaluated and optimized to achieve best possible sensitivity over a broad range of compounds, e.g. polar and nonpolar, volatile and nonvolatile. We explored TDU/CIS parameters by an experimental design approach, chose optimal MRMs for every compound and tested different modifiers to access particle-adsorbed analytes. With the final method we were able to determine around 100 relevant compounds in surface waters in the sub ng/L range. Comprehensive validation data were collected and the method was applied successfully to real world samples. EU-WFD requirements for inland surface water were fulfilled for all included analytes except cypermethrin, heptachlor and heptachlorepoide for which the required LOQs could not be reached.

Limits of Quantification. Limits of quantification and limits of detection were calculated from calibration lines near the expected LOQ as per the requirements of DIN 32645 [8]. If the blank analysis revealed a significant analyte peak, LOQs were determined based on repeat analyses (n=6) of blank samples. At the LOQ, the quantifier/qualifier peak area ratio must be in a range between 80 and 120 % of the expected ratio for at least one qualifier. Furthermore the relative standard deviation (RSD) of repeated analyses at the LOQ level must be below 20 % and the trueness between 80 and 120 %. If these additional specifications were not met at the calculated LOQ the LOQ value was increased to a concentration at which all specifications were met. If feasible, i.e. if the background concentration of an analyte was low, river water was used as matrix when establishing LOQ. For certain compounds like PAHs the background value of the available river water was too high. In these cases either tap or mineral water were used as matrix for LOQ determination. Generally all validation data strongly depend on the level of background contamination and its uniformity. Moreover, the background contamination of the laboratory and skills of the analyst influence the quality of validation data in general.

Table 2 presents LOQs for all analytes also listing the required LOQs from EU-WFD and other legislation. In cases where the EQS refers to a sum of multiple analytes the required LOQ was calculated separately for each of these analytes. This is a very strict interpretation assuming that only one of the

respective analytes is present and all others are not.

The LOQ for cypermethrin of 0.12 ng/L missed the required LOQ of 0.024 ng/L for inland surface waters by a modest factor 5. By employing negative chemical ionization (NCI) instead of EI the required LOQ is likely to be achievable. To date there is presumably no technique available at all to reach the required LOQ of 0.06 pg/L for heptachlor and heptachlorepoide for inland surface waters.

The following chromatograms (figures 5a-q) show representative analyte peaks (quantifier and qualifier MRMs) near their respective LOQs.

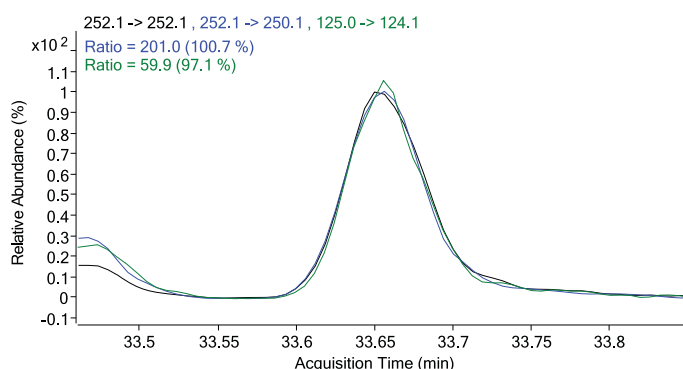


Figure 5a. Benzo[a]pyrene peak at 0.040 ng/L in mineral water. LOQ: 0.033 ng/L.

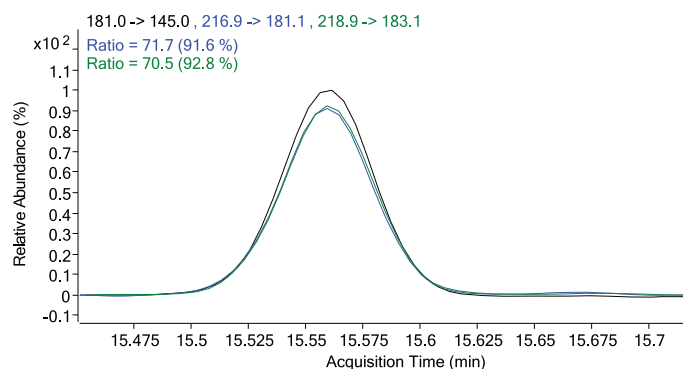


Figure 5b. γ -HCH peak at 0.052 ng/L in mineral water. LOQ: 0.052 ng/L.

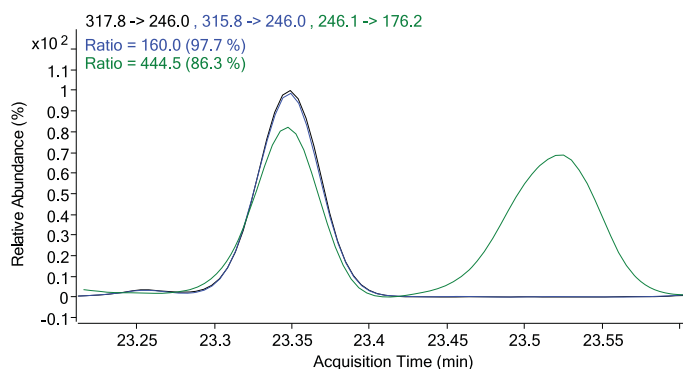


Figure 5c. p,p'-DDE peak at 0.026 ng/L in mineral water. LOQ: 0.017 ng/L.

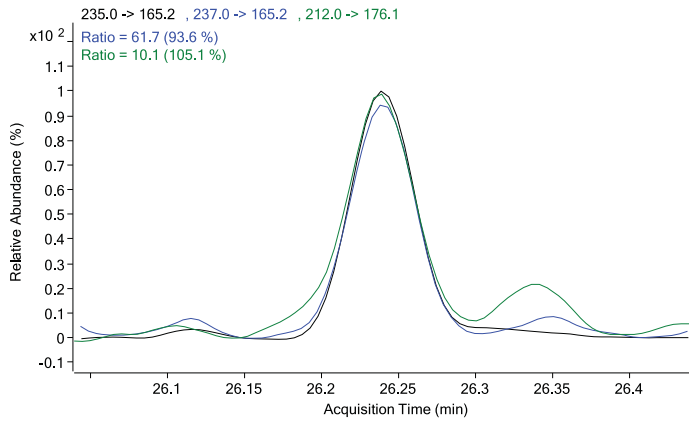


Figure 5d. *p,p'*-DDT Peak at 0.068 ng/L in river water. LOQ: 0.067 ng/L.

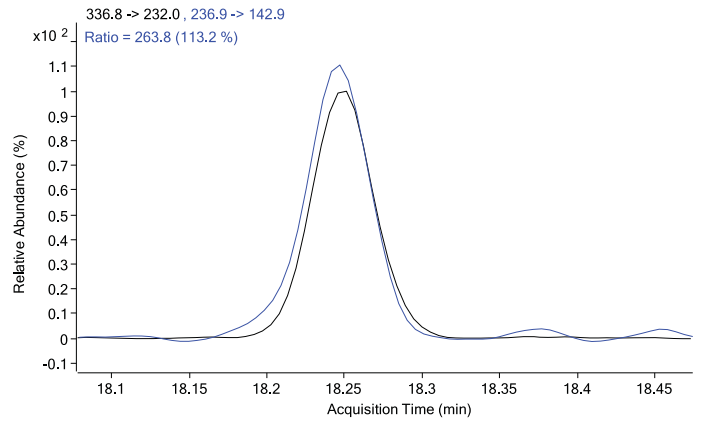


Figure 5e. Heptachlor peak at 0.052 ng/L in river water. LOQ: 0.052 ng/L.

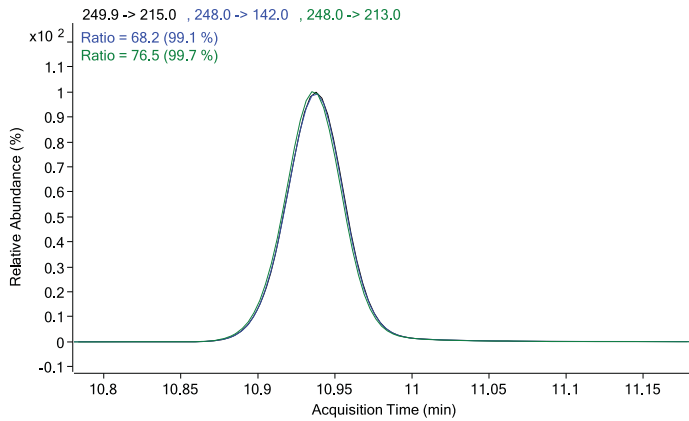


Figure 5f. Pentachlorobenzene peak at 0.16 ng/L in river water. LOQ: 0.075 ng/L.

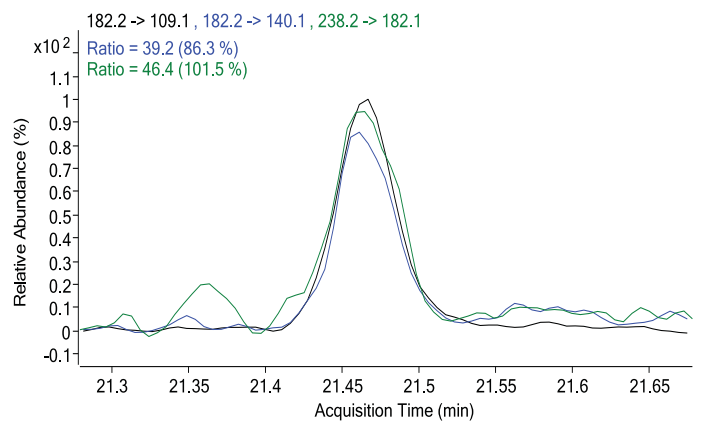


Figure 5g. Cybutryne peak at 0.030 ng/L in mineral water. LOQ: 0.030 ng/L.

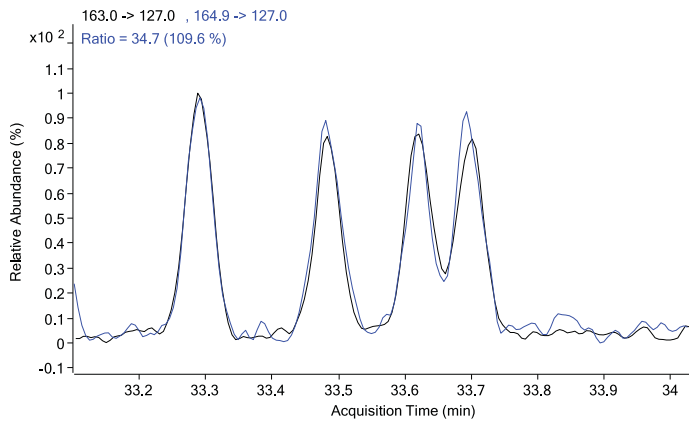


Figure 5h. Cypermethrin peaks at 0.12 ng/L in river water. LOQ: 0.12 ng/L.

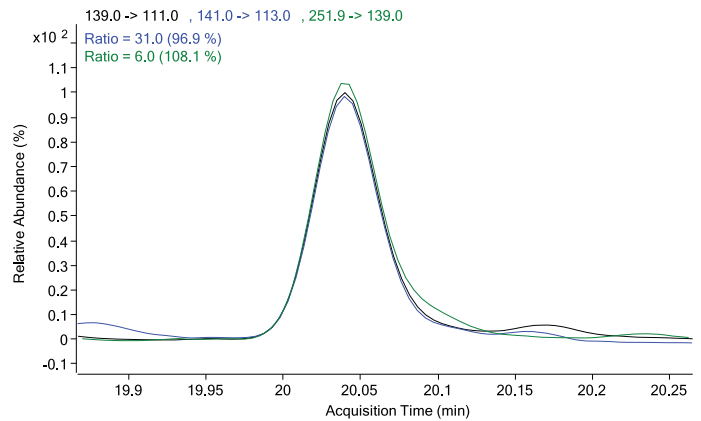


Figure 5i. Dicofol peak at 0.15 ng/L in river water. LOQ: 0.15 ng/L.

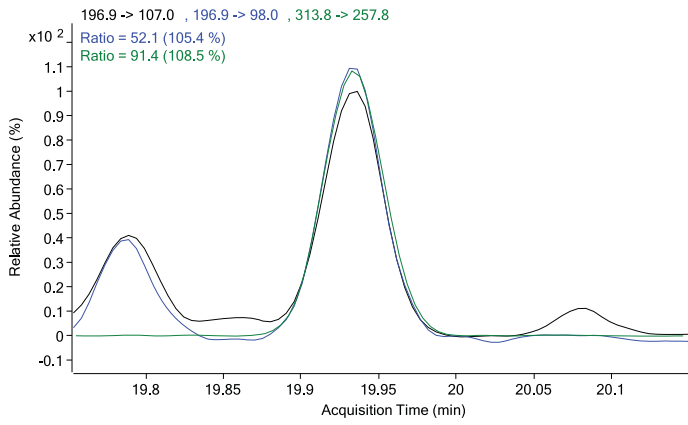


Figure 5j. Chlorpyrifos-ethyl peak at 0.024 ng/L in river water. LOQ: 0.024 ng/L.

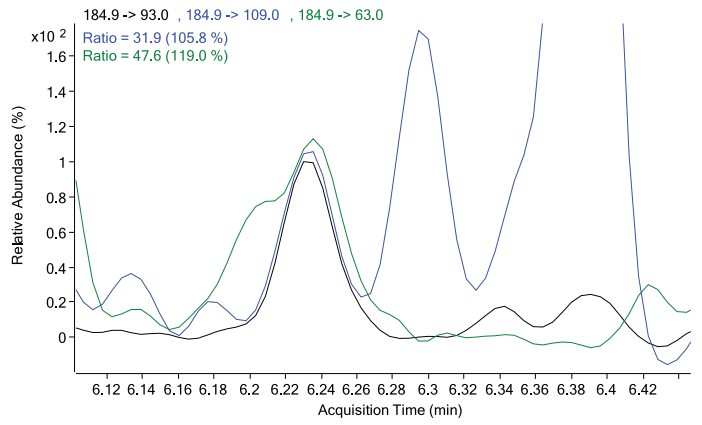


Figure 5k. Dichlorvos peak at 0.073 ng/L in river water. LOQ: 0.073 ng/L.

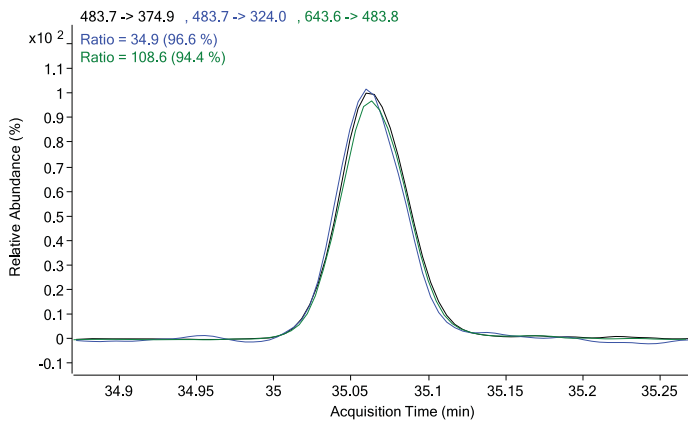


Figure 5l. PBDE 154 peak at 0.021 ng/L in river water. LOQ: 0.020 ng/L.

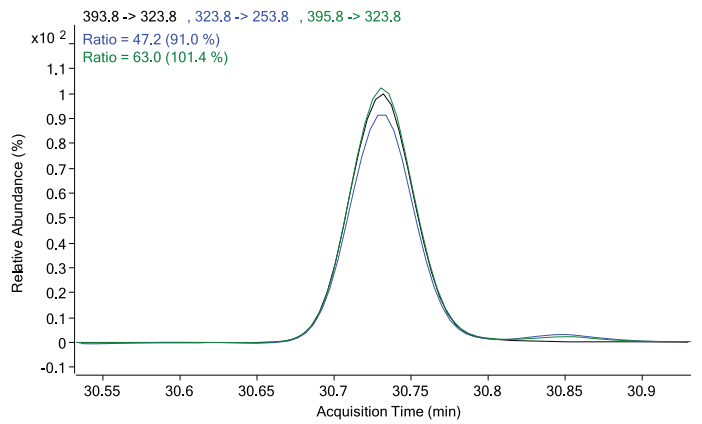


Figure 5m. PCB 189 peak at 0.060 ng/L in river water. LOQ: 0.054 ng/L.

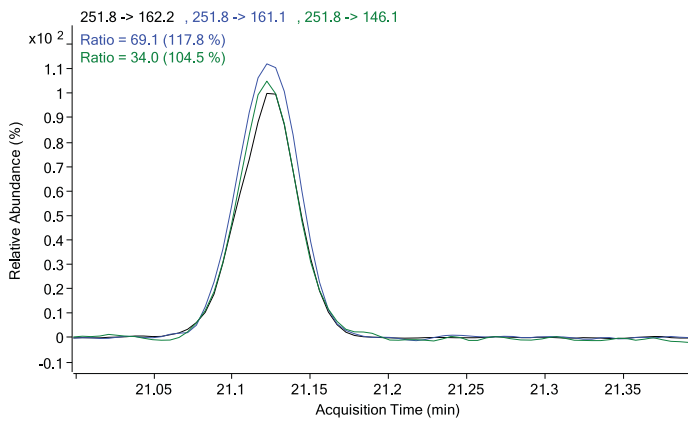


Figure 5n. Pendimethalin peak at 0.10 ng/L in river water. LOQ: 0.094 ng/L.

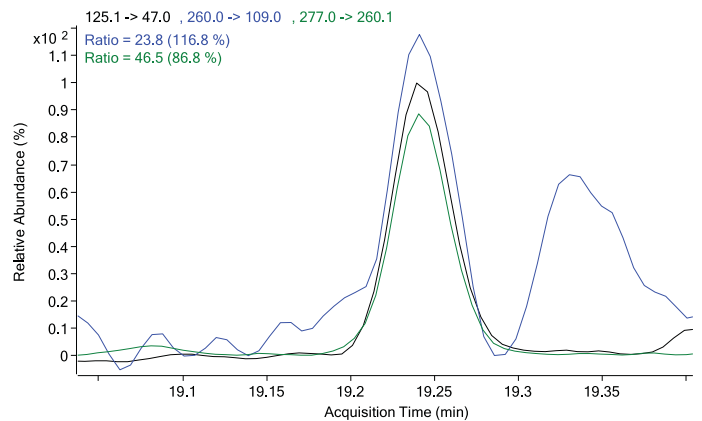


Figure 5o. Fenitrothion peak at 0.027 ng/L in river water. LOQ: 0.024 ng/L.

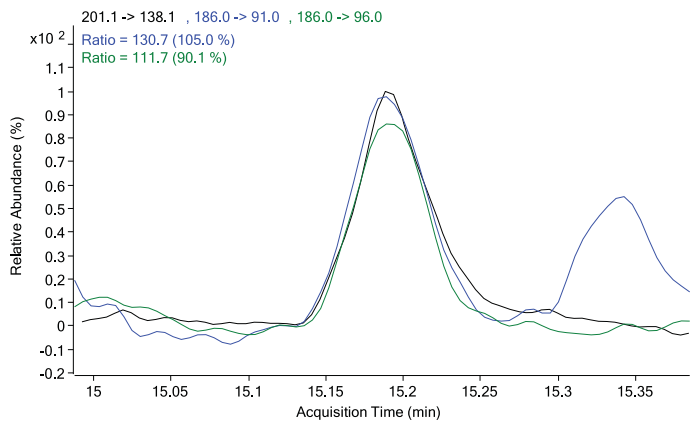


Figure 5p. Simazine peak at 2.4 ng/L in river water. LOQ: 1.9 ng/L.

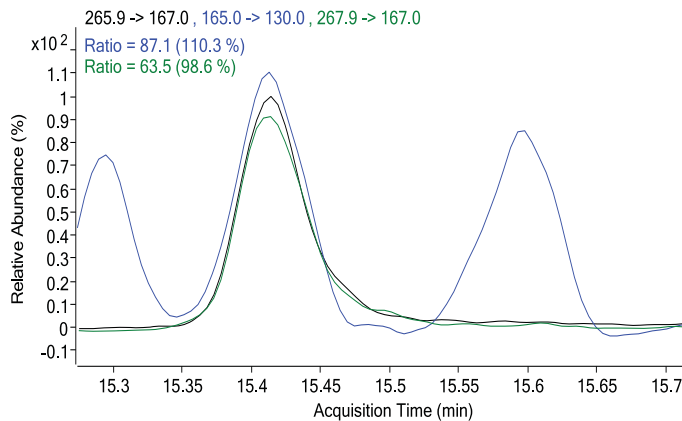


Figure 5q. Pentachlorophenol peak at 6.4 ng/L in mineral water. LOQ: 3.0 ng/L.

Repeatability and Trueness. Repeat analyses (n=6) of mineral water samples spiked at levels close to the respective LOQs revealed relative standard deviations between 1 and 15 % for all compounds with an average of 6.9 %. Trueness was between 90 and 110 % for most analytes.

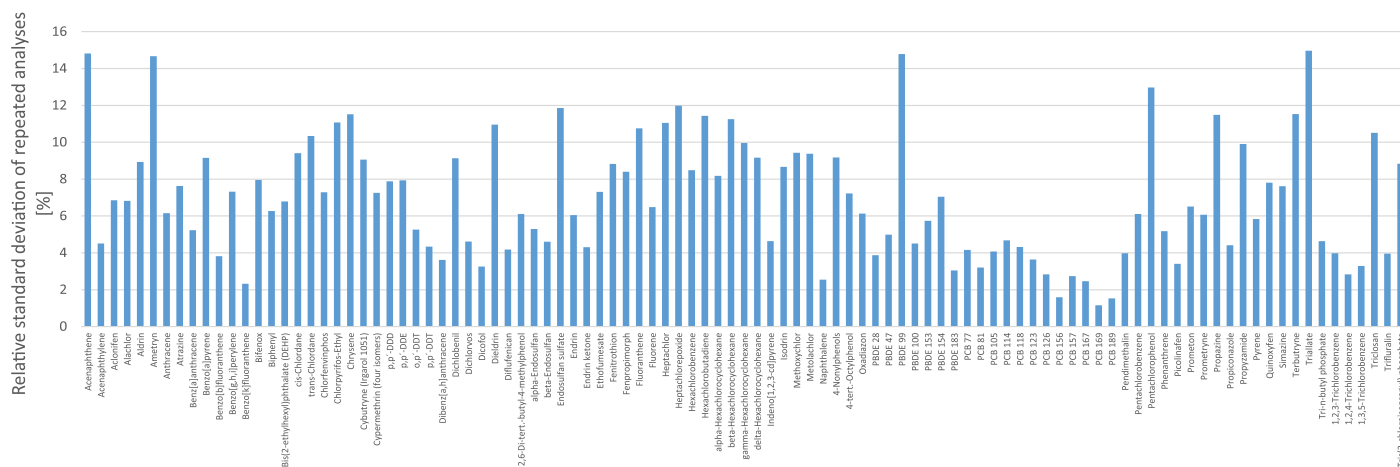


Figure 6. Relative standard deviation of analysis values of spiked mineral water near the respective LOQs (n=6).

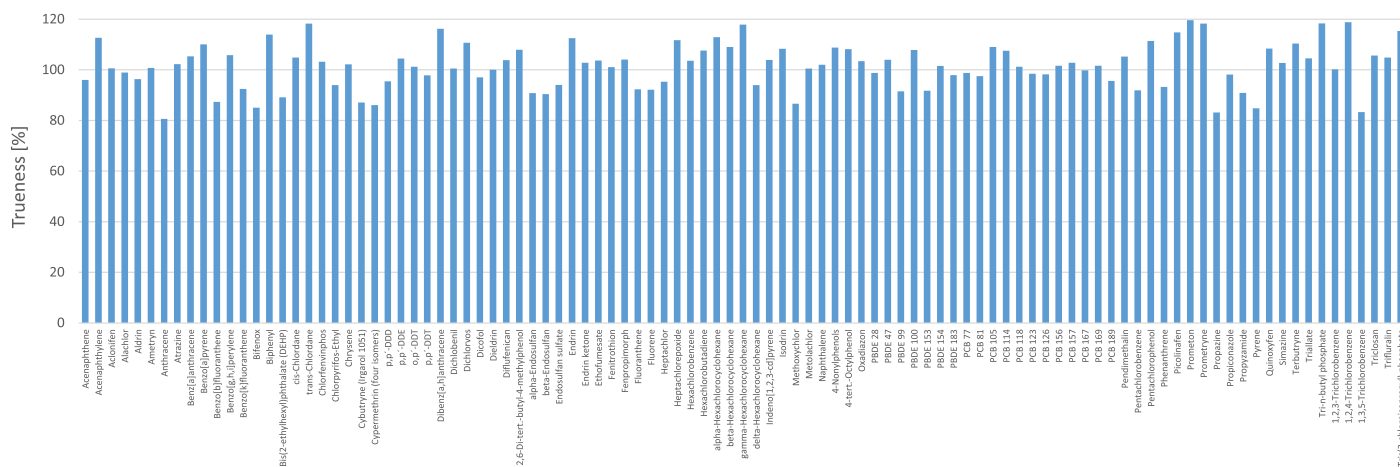


Figure 7. Average trueness of analysis values of spiked mineral water near the respective LOQs (n=6).

Uncertainty of measurement. Relative uncertainty of measurement was calculated from six repeated analyses with the aid of an Excel sheet of the University Stuttgart, Germany (Freeware, © 2015 Dr. M. Koch, Institut für Siedlungswasserbau, Universität Stuttgart, www.aqsbw.de [9]). According to 2009/90/EC [4] the relative uncertainty of measurement at the respective EQS may not exceed 50 % which is fulfilled for analytes from the EU-WFD (Table 3).

Calibration. For the majority of compounds, the calibration range spans up to between 50- and 200-fold their LOQ. Establishing quadratic calibration functions enables this range for many analytes. Besides the expected flattened calibration curves also steepened curves were obtained.

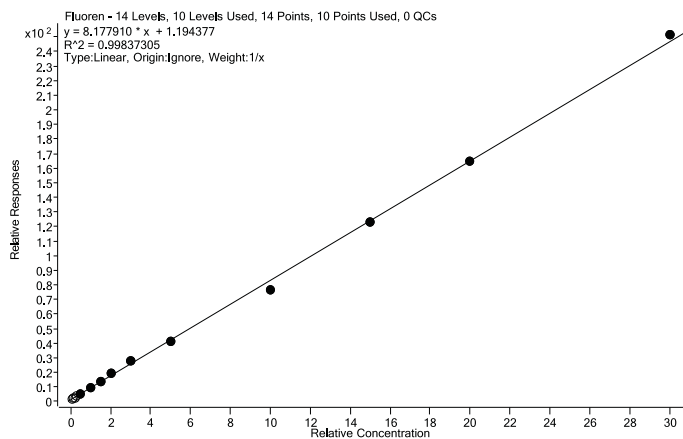


Figure 8a. Linear calibration function for fluorene in the range between 0.5 and 30 ng/L.

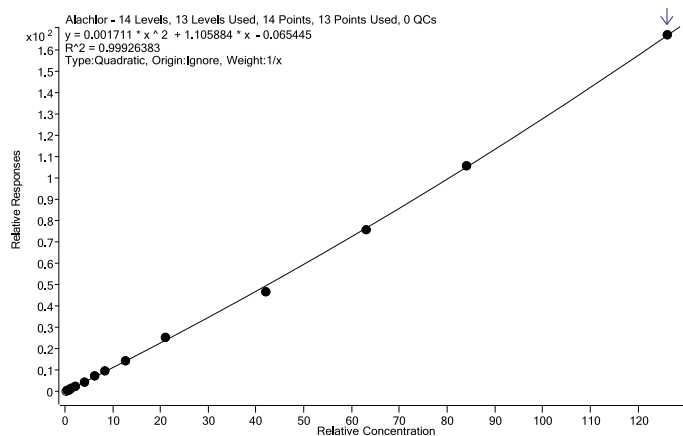


Figure 8b. Steepened quadratic calibration function foralachlor in the range between 0.53 and 126 ng/L.

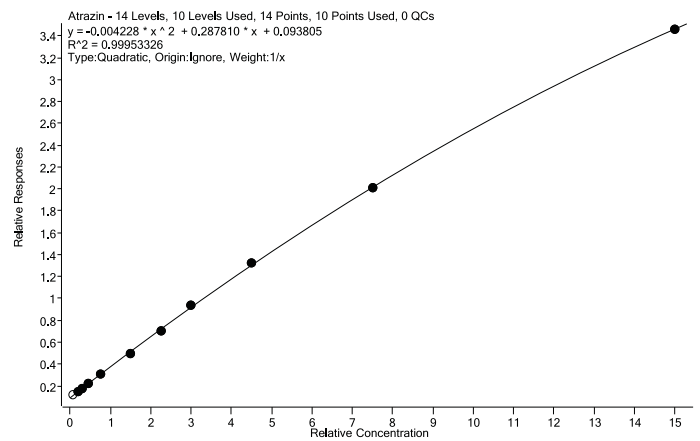


Figure 8c. Flattened quadratic calibration function for atrazine in the range between 0.19 and 15 ng/L.

Quantitation of particle-adsorbed analytes. The correct quantitation of particle-adsorbed compounds like PAHs was examined and confirmed with the aid of certified reference sediment (WEPAL SETOC 745, channel sludge). Analysis results were obtained for PAHs and some OCPs.

Clean tap water samples of 100 mL were spiked with 5, 10 or 15 mg reference sediment and 30 μ L of the internal standard solution. This corresponds to particle content levels of 50, 100 or 150 mg/L, which is a realistic range for real surface water samples.

The average analysis results obtained from four repeated analyses of spiked samples were compared to the theoretical analysis values calculated from the certificate of the sediment. For virtually all compounds, good agreement was achieved. Analysis results for fluorene and benzo[a]pyrene tended to be on the low side, for chrysene the results were on the high side. It is known that chrysene co-elutes with triphenylene on the GC column used and this might help explain the analysis result.

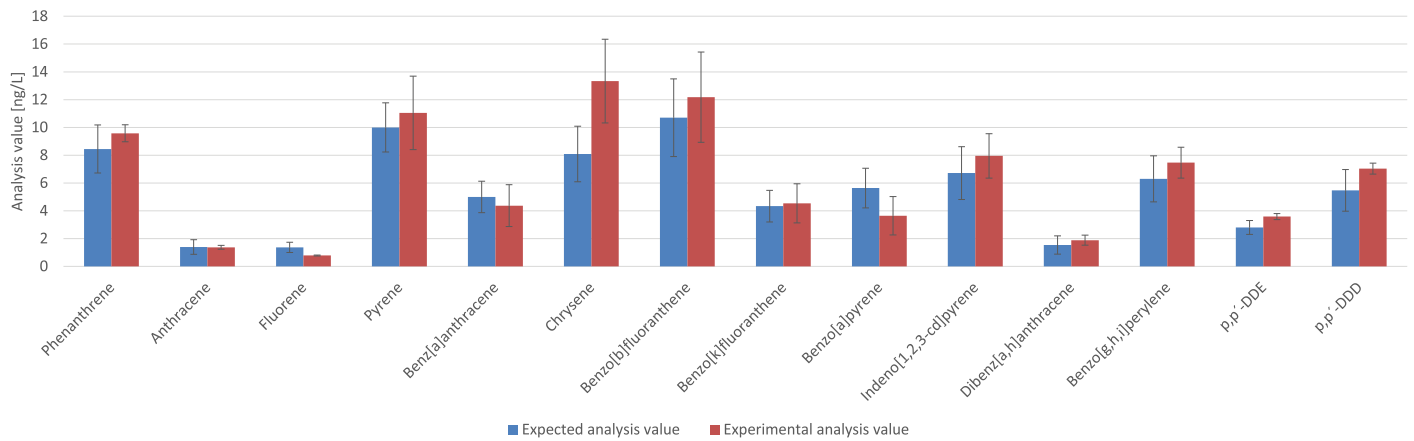


Figure 9a. Quantification of particle-adsorbed analytes shown for a certified reference sediment (WEPAL SETOC 745, channel sludge) at a concentration of 100 mg particles per liter water sample. Comparison between the theoretical analysis values calculated from the certificate and the experimental analysis values. Error bars represent the standard deviation of the measurements.

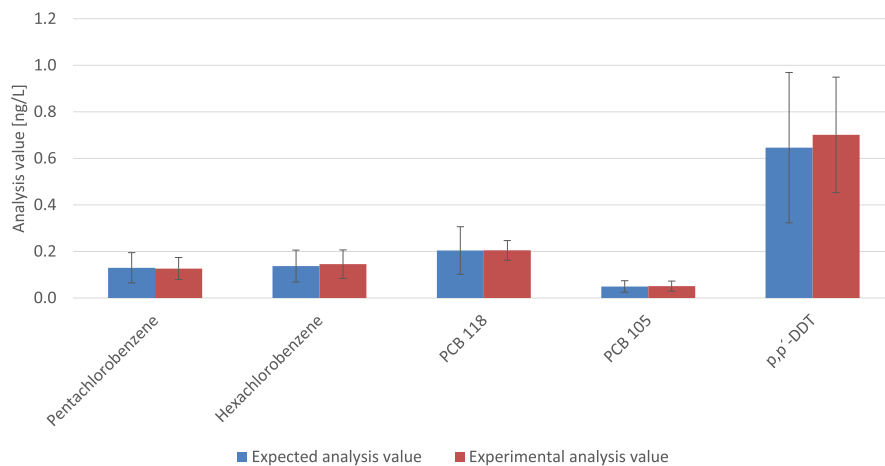


Figure 9b. Quantification of particle-adsorbed analytes shown for a certified reference sediment (WEPAL SETOC 745, channel sludge) at a concentration of 100 mg particles per liter water sample. Comparison between the theoretical analysis values calculated from the certificate and the experimental analysis values. Error bars represent the standard deviation of the measurements.

Application to real samples. Analyses showed good repeatability and in case of samples spiked in an external laboratory the achieved analysis values were in good agreement with the spiked amounts. This can be seen in figure 10 for ground water spiked with a number of pesticides. Performing calibration with this groundwater and application to spiked real water samples yielded analysis values of good trueness for virtually all compounds. In case a compound background concentration was found in the respective water sample, the background concentration was subtracted from the analysis value of the spiked sample. This could lead to less trueness of the experimental

analysis value, e.g. for 4-nonylphenols, 4-octylphenol or tris(2-chloroisopropyl) phosphate (TCPP). In case the background concentration was near or even exceeded the spiked concentration the value was omitted for the respective water sample (missing bar in the diagram), see figure 11.

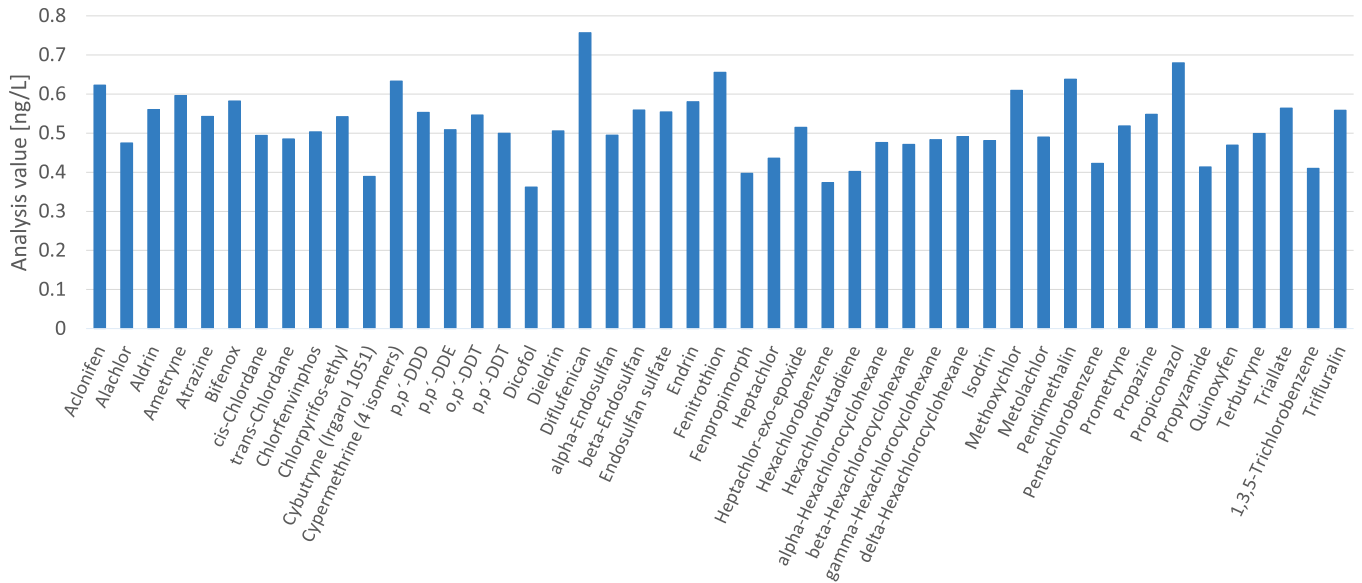


Figure 10. Analysis values for clean ground water spiked with 0.5 ng/L of each shown pesticide. The sample was spiked in a customer`s laboratory with a different standard solution than used for method validation experiments. Calibration samples were prepared in the same ground water.

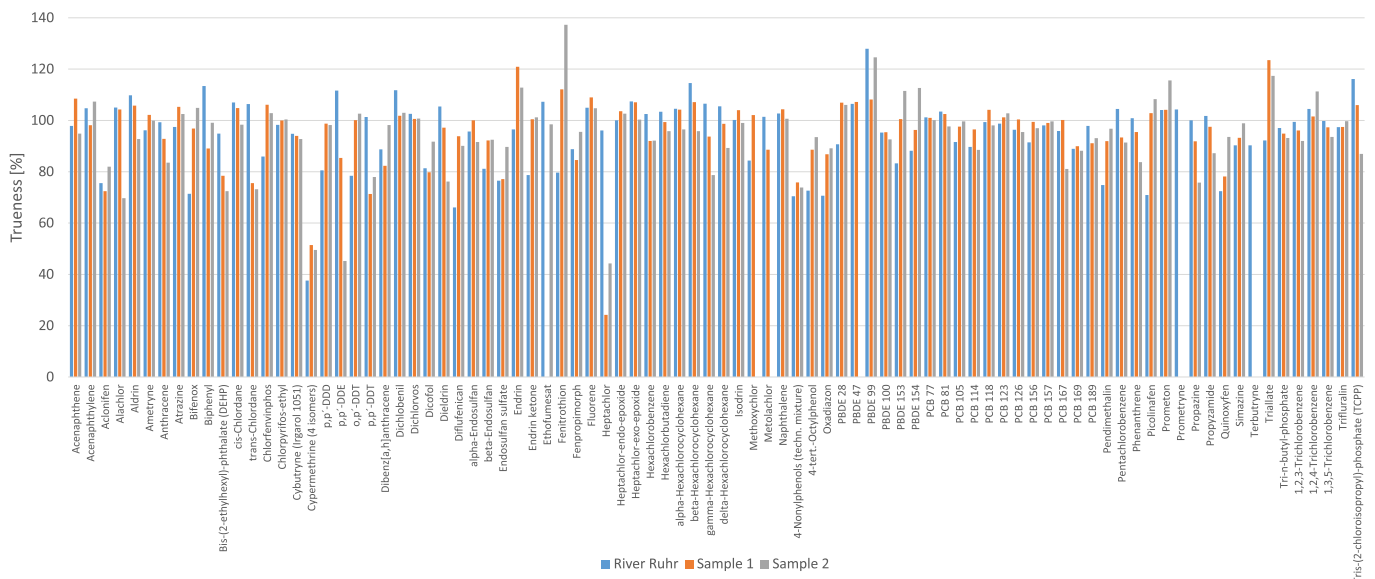


Figure 11. Trueness of analysis values for three different real water samples spiked at medium concentrations (individual for each analyte). Calibration samples were prepared in clean ground water. In case a compound revealed a background concentration in the respective water that concentration was subtracted from the analysis value of the spiked sample. This could lead to less trueness of the experimental analysis value, e.g. for 4-nonylphenols, 4-octylphenol or tris(2-chloroisopropyl) phosphate (TCPP). In case the background concentration was near or even exceeded the spiked concentration the value was omitted for the respective water (missing bar in the diagram).

Real world water samples, e.g. river-, ground-, tap-, mineral water and effluents from sewage treatment plants, could be analyzed without any issues (table 4). For no analyte was a major coelution found on the quantifier ion transition; and each analyte had at least one qualifier ion transition without coelution.

CONCLUSIONS

The developed Twister-TDU-GC-MS/MS method enables the determination of around 100 relevant contaminants from as little as 100 mL surface water sample, including particle-adsorbed compounds, in a single analytical run. The Agilent Technologies 7010 triple quadrupole MS and the GERSTEL Twister represent the ideal combination for reaching LOQs in the low double-digit to low triple-digit pg/L range for the vast majority of analytes. Comprehensive validation data were collected and the method was successfully applied to real world samples. Relative standard deviations laid between 1 and 15 % for all compounds with an average of 6.9 %. Trueness was mainly between 90 and 110 %. Requirements of the EU-WFD for inland surface waters were fulfilled for all analytes with the exception of cypermethrin, heptachlor and heptachlorepoide, for which the required LOQs are extremely low. "Other surface waters" as mentioned by the EU-WFD, such as coastal waters, were not tested with this analysis workflow. The developed method is straightforward, requiring only limited manual work. The method is flexible and can readily be used to determine additional contaminants of relevance for the field of water analysis.

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Table 1. List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
1,3,5-Trichlorobenzene-d ₃	4.50	5.016	185.0 -> 113.0 185.0 -> 149.9	40 25	30 30	2	-
1,3,5-Trichlorobenzene	4.50	5.031	179.9 -> 109.0 179.9 -> 144.9 181.9 -> 144.9	35 25 25	40 40 40	2	1,3,5-Trichlorobenzene-d ₃
1,2,4-Trichlorobenzene	5.20	5.496	179.9 -> 109.0 181.9 -> 74.0 179.9 -> 145.0	30 45 15	40 40 40	2	1,3,5-Trichlorobenzene-d ₃
Naphthalene-d ₈	5.20	5.572	136.1 -> 84.1 136.1 -> 108.1	25 20	10 10	2	-
Naphthalene	5.20	5.608	127.1 -> 51.1 129.1 -> 103.1 127.1 -> 101.1	7 40 40	10 10 10	2	Naphthalene-d ₈
Hexachlorobutadiene	5.77	5.924	224.8 -> 189.9 224.8 -> 154.9 226.9 -> 191.9	15 35 15	50 50 50	2	1,3,5-Trichlorobenzene-d ₃
1,2,3-Trichlorobenzene	5.77	5.930	179.9 -> 109.0 179.9 -> 74.0 181.9 -> 74.0	30 45 45	40 40 40	2	1,3,5-Trichlorobenzene-d ₃
Dichlorvos-d ₆	6.03	6.167	190.9 -> 99.0 190.9 -> 115.0	15 15	10 10	15	-
Dichlorvos	6.03	6.219	184.9 -> 93.0 184.9 -> 109.0 184.9 -> 63.0	10 15 25	80 80	15	Dichlorvos-d ₆
Dichlobenil	7.40	7.750	171.0 -> 100.0 173.0 -> 100.0 171.0 -> 136.1	25 25 15	50 50 50	2	α-Hexachlorocyclohexane-d ₆
Biphenyl	7.40	8.295	155.1 -> 129.1 152.1 -> 126.1 154.1 -> 115.1	30 15 20	10 10 10	2	α-Hexachlorocyclohexane-d ₆
Acenaphthylene	8.68	9.592	152.1 -> 126.0 152.1 -> 102.1 150.1 -> 98.0	30 30 30	50 50 50	10	α-Hexachlorocyclohexane-d ₆
Acenaphthene-d ₁₀	9.85	10.134	162.0 -> 160.1 164.0 -> 162.1	20 15	15 15	10	-
Acenaphthene	9.85	10.222	151.0 -> 149.9 152.1 -> 126.0 152.0 -> 152.0	20 30 20	70 70 70	10	Acenaphthene-d ₁₀
2,6-Di-tert-butyl-4-methylphenol	10.48	10.650	220.1 -> 205.2 205.1 -> 161.1 205.1 -> 145.1	40 40 50	10 10 10	10	α-Hexachlorocyclohexane-d ₆
Pentachlorobenzene	10.48	10.910	249.9 -> 215.0 248.0 -> 142.0 248.0 -> 213.0	20 45 20	60 60 60	10	α-Hexachlorocyclohexane-d ₆
Fluorene	11.18	12.100	165.1 -> 163.1 166.1 -> 165.1 165.1 -> 164.1	35 15 20	30 30 30	10	Phenanthrene-d ₁₀
4-tert-Octylphenol	11.18	12.414	135.1 -> 107.1 135.1 -> 95.1 206.0 -> 107.1 206.0 -> 135.0	50 30 40 12	15 15 15 15	10	α-Hexachlorocyclohexane-d ₆
Tri-n-butyl phosphate	12.88	13.290	211.0 -> 99.0 155.0 -> 81.0 99.0 -> 81.0	50 40 50	10 10 10	2	α-Hexachlorocyclohexane-d ₆

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
Trifluralin-d ₁₄	13.55	13.823	315.0 -> 267.0 266.9 -> 163.1	15 15	20 20	10	-
Trifluralin	13.55	13.986	305.9 -> 264.0 264.0 -> 206.2 264.0 -> 160.1	5 5 15	40 40 40	10	Trifluralin-d ₁₄
α-Hexachlorocyclohexane-d ₆	13.55	14.216	222.0 -> 184.9 222.0 -> 147.9	10 25	7 7	10	-
α-Hexachlorocyclohexane	13.55	14.362	182.9 -> 147.0 180.9 -> 109.0 180.9 -> 145.0	15 30 15	10 10 10	10	α-Hexachlorocyclohexane-d ₆
Hexachlorobenzene	13.55	14.631	283.8 -> 213.9 281.8 -> 211.9 248.9 -> 214.0	30 30 15	10 10 10	10	α-Hexachlorocyclohexane-d ₆
4-Nonylphenols (tech. mixture)	13.55	14.852 (multiple peaks)	107.1 -> 77.0 121.1 -> 91.1 121.1 -> 77.0	50 50 50	7 7 7	10	α-Hexachlorocyclohexane-d ₆
Simazine-d ₅	13.55	15.051	190.9 -> 101.1 187.9 -> 96.0	15 15	7 7	10	-
Simazine	13.55	15.128	201.1 -> 138.1 186.0 -> 91.0 186.0 -> 96.0	10 5 10	10 10 10	10	Simazine-d ₅
Prometon	13.55	15.224	224.9 -> 58.1 210.0 -> 112.1 224.9 -> 168.1	15 15 10	5 5 5	10	Simazine-d ₅
Atrazine	13.55	15.354	214.9 -> 58.1 202.0 -> 122.1 200.0 -> 122.1	10 5 5	10 10 10	10	Simazine-d ₅
β-Hexachlorocyclohexane	13.55	15.402	181.0 -> 145.0 216.9 -> 181.1 218.9 -> 183.1	10 10 10	10 10 10	10	α-Hexachlorocyclohexane-d ₆
Pentachlorophenol- ¹³ C ₆	13.55	15.465	273.8 -> 171.9 171.8 -> 137.0	40 30	7 7	10	-
Pentachlorophenol	13.55	15.476	265.9 -> 167.0 165.0 -> 130.0 267.9 -> 167.0	25 25 25	10 10 10	10	Pentachlorophenol- ¹³ C ₆
Propazine	13.55	15.537	229.1 -> 58.1 214.2 -> 94.1 214.2 -> 172.2	10 20 10	5 5 5	10	Simazine-d ₅
γ-Hexachlorocyclohexane	13.55	15.607	181.0 -> 145.0 216.9 -> 181.1 218.9 -> 183.1	10 10 10	10 10 10	10	α-Hexachlorocyclohexane-d ₆
Phenanthrene-d ₁₀	15.72	15.858	188.0 -> 186.1 188.0 -> 160.1	25 30	10 10	2	-
Phenanthrene	15.72	15.948	178.1 -> 152.1 178.1 -> 151.1 176.1 -> 150.1	30 50 30	10 10 10	2	Phenanthrene-d ₁₀
Propyzamide	15.72	16.021	173.0 -> 109.0 145.0 -> 109.0 145.0 -> 74.0	30 10 30	10 10 10	2	Trifluralin-d ₁₄
Anthracene	15.72	16.135	178.1 -> 152.1 178.1 -> 151.1 176.1 -> 150.1	30 50 30	10 10 10	2	Phenanthrene-d ₁₀

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
δ -Hexachlorocyclohexane	15.72	16.542	181.1 -> 145.1 217.0 -> 181.1 219.0 -> 183.1	15 5 5	30 30 30	2	α -Hexachlorocyclohexane-d ₆
Tris(2-chloroisopropyl) phosphate (TCPP)	15.72	16.548 (two peaks)	276.9 -> 125.0 278.9 -> 125.0 201.0 -> 125.0	40 40 30	7 7 7	2	Alachlor-d ₁₃
Triallate	15.72	16.854	268.0 -> 184.1 142.9 -> 83.0 270.0 -> 186.1	20 15 20	15 15 15	2	Phenanthrene-d ₁₀
Alachlor-d ₁₃	17.80	18.240	200.0 -> 138.1 251.0 -> 91.0	30 15	5 5	40	-
Heptachlor	17.80	18.305	336.8 -> 232.0 236.9 -> 118.8 236.9 -> 142.9	40 25 25	40 80 120	40	Alachlor-d ₁₃
Alachlor	17.80	18.426	237.0 -> 160.1 188.1 -> 160.2 188.1 -> 132.1	5 10 15	10 10 10	40	Alachlor-d ₁₃
Ametryne	17.80	18.472	227.0 -> 58.1 212.0 -> 122.1 212.0 -> 94.0	10 10 20	5 5 5	40	Simazine-d ₅
Prometryne	17.80	18.631	241.0 -> 184.2 226.0 -> 184.2 241.0 -> 58.2	10 10 10	5 5 5	40	Alachlor-d ₁₃
Terbutryne	18.90	19.095	226.2 -> 96.1 185.0 -> 170.1 241.1 -> 170.2	20 5 15	30 30 30	10	Chlorpyrifos-ethyl-d ₁₀
Fenitrothion	18.90	19.174	125.1 -> 47.0 260.0 -> 109.0 277.0 -> 260.1	15 15 5	30 30 30	10	Chlorpyrifos-ethyl-d ₁₀
Ethofumesate	18.90	19.317	285.9 -> 207.1 206.9 -> 137.2 206.9 -> 161.1	5 10 5	30 30 30	10	Chlorpyrifos-ethyl-d ₁₀
Aldrin	19.47	19.584	254.9 -> 220.0 262.9 -> 190.9 262.9 -> 192.9	20 35 35	20 20 20	10	PCB 111- ¹³ C ₁₂
Metolachlor	19.47	19.783	238.0 -> 162.2 238.0 -> 133.2 240.0 -> 162.2	10 30 10	20 20 20	10	Chlorpyrifos-ethyl-d ₁₀
Chlorpyrifos-ethyl-d ₁₀	19.47	19.836	323.9 -> 259.9 259.8 -> 166.9	15 30	10 10	10	-
Fenpropimorph	19.47	19.973	302.9 -> 128.0 128.1 -> 86.1 128.1 -> 70.1	5 10 10	10 10 10	10	Chlorpyrifos-ethyl-d ₁₀
Chlorpyrifos-ethyl	19.47	19.982	196.9 -> 107.0 196.9 -> 98.0 313.8 -> 257.8	40 30 15	10 10 10	10	Chlorpyrifos-ethyl-d ₁₀
Dicofol	19.47	20.003	139.0 -> 111.0 141.0 -> 113.0 251.9 -> 141.0	18 18 18	20 20 20	10	Chlorpyrifos-ethyl-d ₁₀
Isodrin	20.35	20.652	193.0 -> 157.0 195.0 -> 123.0 193.0 -> 123.0	20 30 30	5 5 5	10	PCB 70- ¹³ C ₁₂

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
Heptachlor-exo-epoxide	20.35	21.084	288.8 -> 253.0 288.8 -> 217.0 182.9 -> 118.9	15 35 25	90 50 90	10	PCB 70- ¹³ C ₁₂
Pendimethalin	20.35	21.173	251.8 -> 162.2 251.8 -> 161.1 251.8 -> 146.1	10 15 20	5 5 5	10	Trifluralin-d ₁₄
Fluoranthene	20.35	21.212	202.1 -> 176.0 202.1 -> 152.1 200.1 -> 174.0	40 40 40	5 5 5	10	PCB 70- ¹³ C ₁₂
Heptachlor-endo-epoxide	20.35	21.254	288.8 -> 253.0 288.8 -> 217.0 182.9 -> 118.9	15 35 25	90 50 90	10	PCB 70- ¹³ C ₁₂
PCB 70- ¹³ C ₁₂	20.35	21.299	301.8 -> 232.0 303.8 -> 234.0	40 40	5 5	10	-
Chlorfenvinphos	20.35	21.369 (two peaks)	266.9 -> 159.1 268.9 -> 161.0 322.8 -> 266.8	15 15 10	5 5 5	10	Chlorpyrifos-ethyl-d ₁₀
Cybutryne (Irgarol 1051)	20.35	21.512	182.2 -> 109.1 182.2 -> 140.1 238.2 -> 182.1	10 10 10	5 5 5	10	Chlorpyrifos-ethyl-d ₁₀
trans-Chlordane	21.75	21.974	372.9 -> 300.9 236.9 -> 118.9 271.9 -> 236.9	10 30 15	20 20 20	10	PCB 111- ¹³ C ₁₂
Triclosan	21.75	22.023	218.1 -> 155.1 287.9 -> 145.9 287.9 -> 218.0	25 20 20	20 20 20	10	p,p'-DDT-d ₈
Pyrene	21.75	22.153	202.1 -> 151.0 200.1 -> 150.0 202.1 -> 175.0	50 40 50	15 15 15	10	PCB 70- ¹³ C ₁₂
α-Endosulfan	21.75	22.409	194.9 -> 159.0 194.9 -> 125.0 194.9 -> 160.0	5 20 5	45 45 45	10	PCB 70- ¹³ C ₁₂
cis-Chlordane	21.75	22.536	372.9 -> 300.9 236.9 -> 118.9 271.9 -> 236.9	10 30 15	20 20 20	10	PCB 111- ¹³ C ₁₂
PCB 111- ¹³ C ₁₂	22.80	23.207	335.8 -> 266.0 265.9 -> 230.9	30 30	10 10	5	-
PCB 81	22.80	23.280	289.9 -> 219.9 291.9 -> 219.9 291.9 -> 221.9	30 30 30	30 30 30	5	PCB 111- ¹³ C ₁₂
Dieldrin	22.80	23.362	262.9 -> 193.0 262.9 -> 191.0 237.0 -> 142.9	35 35 25	30 30 30	5	PCB 111- ¹³ C ₁₂
p,p'-DDE	22.80	23.390	317.8 -> 246.0 315.8 -> 246.0 246.1 -> 176.2	15 15 30	20 20 20	5	PCB 111- ¹³ C ₁₂
Oxadiazon	22.80	23.638	174.9 -> 112.0 257.8 -> 112.0 176.9 -> 112.0	15 30 15	10 10 10	5	PCB 111- ¹³ C ₁₂
PCB 77	22.80	23.640	289.9 -> 219.9 291.9 -> 219.9 291.9 -> 221.9	30 30 30	30 30 30	5	PCB 111- ¹³ C ₁₂

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
Endrin	23.90	24.138	262.8 -> 227.9 244.8 -> 173.0 244.8 -> 210.0	20 30 10	100 100 100	10	PCB 111- ¹³ C ₁₂
β-Endosulfan	24.30	24.481	206.9 -> 172.0 236.8 -> 118.8 194.9 -> 124.9	15 30 25	30 30 30	10	PCB 111- ¹³ C ₁₂
PCB 123	24.30	24.498	325.9 -> 255.9 255.9 -> 184.0 325.9 -> 253.9	25 35 25	30 30 30	10	PCB 111- ¹³ C ₁₂
PCB 118	24.30	24.577	325.9 -> 255.9 255.9 -> 184.0 325.9 -> 253.9	25 35 25	30 30 30	10	PCB 111- ¹³ C ₁₂
PBDE 28	24.30	24.627	407.8 -> 248.1 405.8 -> 167.1 405.8 -> 246.0	22 25 20	30 30 30	10	PCB 111- ¹³ C ₁₂
p,p'-DDD	24.77	24.895	234.9 -> 165.1 236.9 -> 165.2 234.9 -> 199.1	20 20 15	25 25 25	10	PCB 111- ¹³ C ₁₂
Aclonifen	24.77	24.906	212.1 -> 182.2 264.1 -> 194.2 264.1 -> 77.1	10 15 35	25 25 25	10	p,p'-DDT-d ₈
PCB 114	24.77	24.976	325.9 -> 255.9 327.9 -> 257.9 327.9 -> 255.9	25 25 25	25 25 25	10	PCB 138- ¹³ C ₁₂
o,p'-DDT	24.77	25.004	234.9 -> 199.1 234.9 -> 165.1 236.9 -> 165.2	15 20 20	25 25 25	10	PCB 138- ¹³ C ₁₂
PCB 105	25.36	25.524	325.9 -> 255.9 255.9 -> 184.0 325.9 -> 253.9	30 35 30	50 50 50	10	PCB 138- ¹³ C ₁₂
Quinoxifen	25.85	25.996	271.9 -> 208.0 308.8 -> 237.0 306.8 -> 271.9	40 20 5	20 20 20	10	Chlorpyrifos-ethyl-d ₁₀
Endosulfan sulfate	25.85	26.039	386.6 -> 288.7 273.8 -> 238.9 271.9 -> 235.0	5 15 15	20 20 20	10	Chlorpyrifos-ethyl-d ₁₀
p,p'-DDT-d ₈	25.85	26.141	242.9 -> 173.1 244.9 -> 173.1	30 30	10 10	10	-
p,p'-DDT	25.85	26.226	235.0 -> 165.2 212.0 -> 176.1 237.0 -> 165.2	20 30 20	30 30 30	10	p,p'-DDT-d ₈
Propiconazole	25.85	26.299 (two peaks)	258.8 -> 69.0 258.8 -> 172.9 260.8 -> 69.0	10 15 10	10 10 10	10	PCB 138- ¹³ C ₁₂
PCB 138- ¹³ C ₁₂	25.85	26.361	371.9 -> 336.9 371.9 -> 301.8	10 30	10 10	10	-
PCB 178- ¹³ C ₁₂	26.55	26.660	405.8 -> 370.9 405.8 -> 335.9	10 40	10 10	10	-
PCB 126	26.55	26.676	325.9 -> 255.9 255.9 -> 184.0 325.9 -> 253.9	25 35 25	35 35 35	10	PCB 178- ¹³ C ₁₂
Diflufenican	26.55	27.024	393.9 -> 265.9 218.0 -> 140.1 266.0 -> 246.1	10 20 15	15 15 15	10	PBDE 100- ¹³ C ₁₂

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
PCB 167	26.55	27.359	359.9 -> 289.9 289.9 -> 219.9 359.9 -> 287.8	25 35 30	35 35 35	10	PCB 178- ¹³ C ₁₂
Endrin ketone	27.54	27.651	316.8 -> 100.8 316.8 -> 280.7 280.9 -> 244.8	10 5 10	30 30 30	2	PCB 138- ¹³ C ₁₂
Benz[a]anthracene-d ₁₂	27.54	27.682	240.2 -> 236.2 240.2 -> 238.2	50 30	10 10	2	-
Benz[a]anthracene	27.54	27.773	228.1 -> 226.1 226.1 -> 224.1 228.1 -> 202.1	40 30 40	15 15 15	2	Benz[a]anthracene-d ₁₂
Chrysene-d ₁₂	27.54	27.833	240.2 -> 236.2 240.2 -> 238.2	50 30	10 10	2	-
Chrysene	27.54	27.948	228.1 -> 226.1 226.1 -> 224.1 228.1 -> 202.1	40 40 40	15 15 15	2	Chrysene-d ₁₂
PCB 156	27.54	28.156	359.9 -> 289.9 289.9 -> 219.9 359.9 -> 287.8	30 35 30	20 20 20	2	PCB 178- ¹³ C ₁₂
Picolinafen	27.54	28.203	376.0 -> 238.1 145.1 -> 95.0 376.0 -> 239.1	20 15 10	20 20 20	2	PBDE 100- ¹³ C ₁₂
Methoxychlor	27.54	28.322	227.0 -> 141.1 227.0 -> 169.1 227.0 -> 212.1	40 25 15	20 20 20	2	PBDE 100- ¹³ C ₁₂
PCB 157	27.54	28.354	359.9 -> 289.9 289.9 -> 219.9 359.9 -> 287.8	30 35 30	20 20 20	2	PCB 178- ¹³ C ₁₂
Bifenox	28.51	28.696	340.9 -> 309.9 340.9 -> 280.9 342.9 -> 311.9	10 15 10	50 50 50	10	PBDE 100- ¹³ C ₁₂
PBDE 47	28.51	28.826	325.8 -> 137.9 325.8 -> 216.8 485.7 -> 325.7	50 30 20	50 50 50	10	PBDE 100- ¹³ C ₁₂
Bis-(2-ethylhexyl) phthalate (DEHP)	29.10	29.266	279.0 -> 148.9 113.0 -> 57.1 113.0 -> 71.1	50 30 25	5 5 5	2	PCB 178- ¹³ C ₁₂
PCB 169	29.10	29.446	359.9 -> 289.9 289.9 -> 219.9 359.9 -> 287.8	30 35 30	90 90 90	2	PCB 178- ¹³ C ₁₂
PCB 189	30.00	30.717	393.8 -> 323.8 323.8 -> 253.8 395.8 -> 323.8	30 35 30	100 100 100	10	PCB 178- ¹³ C ₁₂
PBDE 100- ¹³ C ₁₂	31.20	31.843	575.8 -> 415.9 577.8 -> 417.9	30 30	10 10	20	-
PBDE 100	31.20	31.854	563.6 -> 403.7 403.7 -> 296.7 565.6 -> 405.6	20 30 20	50 50 50	20	PBDE 100- ¹³ C ₁₂
Benzo[b]fluoranthene	32.25	32.473	253.1 -> 251.1 250.1 -> 248.1 252.1 -> 250.1	50 50 50	50 50 50	2	PCB 178- ¹³ C ₁₂
Benzo[k]fluoranthene	32.25	32.576	253.1 -> 251.1 250.1 -> 248.1 252.1 -> 250.1	50 50 50	50 50 50	2	PCB 178- ¹³ C ₁₂

Table 1 (cont.). List of compounds with their respective analysis method details and retention times.

Compound	Time segment [min]	Ret. time [min]	MRM [m/z]	Collision energy [V]	Dwell time [ms]	Gain factor	Internal standard
PBDE 99	32.25	32.690	563.6 -> 403.7 405.8 -> 296.7 403.7 -> 243.7	20 35 35	50 50 50	2	Benzo[a]pyrene-d ₁₂
Cypermethrin (4 isomers)	33.00	33.493 (four peaks)	164.9 -> 127.0 163.0 -> 127.0	5 5	240 80	80	PBDE 100- ¹³ C ₁₂
Benzo[a]pyrene-d ₁₂	33.00	33.612	264.2 -> 260.2 264.2 -> 262.2	40 30	10 10	80	-
Benzo[a]pyrene	33.00	33.700	252.1 -> 252.1 252.1 -> 250.1 125.0 -> 124.1	40 50 15	10 10 10	80	Benzo[a]pyrene-d ₁₂
Perylene-d ₁₂	33.00	33.939	264.2 -> 260.2 264.2 -> 262.2	40 30	10 10	80	-
PBDE 154	34.50	35.058	483.7 -> 374.9 483.7 -> 324.0 643.6 -> 483.8	40 35 20	100 100 100	10	Benzo[a]pyrene-d ₁₂
PBDE 153	35.80	36.179	483.7 -> 323.6 485.7 -> 376.6 643.6 -> 483.6	40 35 20	100 100 100	10	Benzo[a]pyrene-d ₁₂
Indeno[1,2,3-cd]pyrene	37.00	37.807	276.1 -> 274.1 138.1 -> 137.1 276.1 -> 276.1	50 20 40	60 60 60	10	PBDE 183- ¹³ C ₁₂
Dibenz[a,h]anthracene	37.00	37.963	278.1 -> 278.1 278.1 -> 276.1 138.1 -> 137.1	30 50 20	60 60 60	10	PBDE 183- ¹³ C ₁₂
Benzo[g,h,i]perylene	38.35	38.598	276.1 -> 276.1 276.1 -> 274.1 138.0 -> 137.0	40 45 15	15 15 15	10	PBDE 183- ¹³ C ₁₂
PBDE 183- ¹³ C ₁₂	38.35	39.503	575.8 -> 465.8 575.8 -> 494.6	30 30	10 10	10	-
PBDE 183	38.35	39.509	561.9 -> 454.4 561.7 -> 454.9 721.8 -> 561.7	30 45 30	50 50 50	10	PBDE 183- ¹³ C ₁₂

Table 2. Established LOQs for all analytes compared to required LOQs derived from 2013/39/EU, OGeWV or Commission Implementing Decision (EU) 2015/495.

Analyte	LOQ [ng/L]	Required LOQ for „inland surface waters“ and „other surface waters“ [ng/L] ¹	Matrix
Acenaphthene	1.0	N/A	Mineral water
Acenaphthylene	0.10	N/A	Tap water
Aclonifen	0.56	36 3.6	River water
Alachlor	0.42	90 90	River water
Aldrin	0.066	3 ² 1.5 ²	River water
Ametryn	0.069	150	Tap water
Anthracene	0.061	30 30	Mineral water
Atrazine	0.18	180 180	Tap water
Benz[a]anthracene	0.076	N/A	Tap water
Benzo[a]pyrene	0.033	0.051 0.051	Mineral water
Benzo[b]fluoranthene	0.078	5.1 ³ 5.1 ³	Tap water
Benzo[g,h,i]perylene	0.049	2.46 ³ 0.246 ³	Mineral water
Benzo[k]fluoranthene	0.081	5.1 ³ 5.1 ³	Tap water
Bifenox	0.47	3.6 0.36	River water
Biphenyl	9.0	300	Tap water
Bis(2-ethylhexyl) phthalate (DEHP)	80	390 390	Tap water
cis-Chlordane	0.052	0.9	River water
trans-Chlordane	0.026	0.9	River water
Chlorfenvinphos	0.084	30 30	River water
Chlorpyrifos-ethyl	0.024	9 9	River water
Chrysene	0.027	N/A	Mineral water
Cybutryne (Irgarol 1051)	0.030	0.75 0.75	Tap water
Cypermethrin (4 isomers)	0.12	0.024 0.0024	River water
p,p'-DDD	0.020	7.5 ⁴ 7.5 ⁴	Tap water
p,p'-DDE	0.017	7.5 ⁴ 7.5 ⁴	Tap water
o,p'-DDT	0.052	7.5 ⁴ 7.5 ⁴	River water
p,p'-DDT	0.067	7.5 ⁴ 7.5 ⁴	River water
Dibenz[a,h]anthracene	0.073	N/A	Mineral water
Dichlobenil	2.1	N/A	Mineral water

Table 2 (cont.). Established LOQs for all analytes compared to required LOQs derived from 2013/39/EU, OGeV or Commission Implementing Decision (EU) 2015/495.

Analyte	LOQ [ng/L]	Required LOQ for „inland surface waters“ and „other surface waters“ [ng/L] ¹	Matrix
Dichlorvos	0.073	0.18 0.018	River water
Dicofol	0.15	0.39 0.0039	River water
Dieldrin	0.034	3 ² 1.5 ²	Tap water
Diflufenican	0.16	2.7	Tap water
2,6-Di-tert.-butyl-4-methylphenol	5.9	3160	Tap water
α-Endosulfan	0.070	1.5 ⁵ 0.15 ⁵	River water
β-Endosulfan	0.059	1.5 ⁵ 0.15 ⁵	River water
Endosulfan sulfate	0.052	N/A	Tap water
Endrin	0.043	3 ² 1.5 ²	River water
Endrin ketone	0.052	N/A	River water
Ethofumesate	0.073	N/A	Tap water
Fenitrothion	0.024	2.7	River water
Fenpropimorph	0.13	N/A	Tap water
Fluoranthene	0.45	1.89 1.89	Mineral water
Fluorene	0.45	N/A	Mineral water
Heptachlor	0.052	0.00006 0.000003	River water
Heptachlor-endo-epoxide	0.052	0.00006 0.000003	River water
Hexachlorobenzene	0.10	15 ³ 15 ³	River water
Hexachlorobutadiene	0.043	180 ³ 180 ³	Tap water
α-Hexachlorocyclohexane	0.052	6 ⁶ 0.6 ⁶	Tap water
β-Hexachlorocyclohexane	0.13	6 ⁶ 0.6 ⁶	Tap water
γ-Hexachlorocyclohexane	0.052	6 ⁶ 0.6 ⁶	Tap water
δ-Hexachlorocyclohexane	0.052	6 ⁶ 0.6 ⁶	Tap water
Indeno[1,2,3-cd]pyrene	0.044	N/A	Mineral water
Isodrin	0.16	3 ² 1.5 ²	River water
Methoxychlor	0.083	N/A	Tap water
Metolachlor	0.064	60	Tap water
Naphthalene	5.0	600 600	Mineral water
4-Nonylphenols	8.8	90 90	Mineral water

Table 2 (cont.). Established LOQs for all analytes compared to required LOQs derived from 2013/39/EU, OGeV or Commission Implementing Decision (EU) 2015/495.

Analyte	LOQ [ng/L]	Required LOQ for „inland surface waters“ and „other surface waters“ [ng/L] ¹	Matrix
4-tert.-Octylphenol	0.46	30 3	Mineral water
Oxadiazon	0.082	88	Tap water
PBDE 28	0.018	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 47	0.015	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 99	0.050	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 100	0.011	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 153	0.032	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 154	0.020	42 ^{3,7} 4.2 ^{3,7}	River water
PBDE 183	0.13	N/A	River water
PCB 77	0.041	N/A	River water
PCB 81	0.039	N/A	River water
PCB 105	0.043	N/A	River water
PCB 114	0.036	N/A	River water
PCB 118	0.012	N/A	Tap water
PCB 123	0.037	N/A	River water
PCB 126	0.050	N/A	River water
PCB 156	0.046	N/A	River water
PCB 157	0.047	N/A	River water
PCB 167	0.044	N/A	River water
PCB 169	0.054	N/A	River water
PCB 189	0.054	N/A	River water
Pendimethalin	0.094	N/A	River water
Pentachlorobenzene	0.075	2.1 0.21	River water
Pentachlorophenol	3.0	120 120	Mineral water
Phenanthrene	2.5	150	Mineral water
Picolinafen	0.26	2.1	River water
Prometon	0.18	N/A	River water
Prometryne	0.23	150	Tap water
Propazine	0.057	N/A	Tap water
Propiconazole	0.14	300	Tap water
Propyzamide	0.35	N/A	Tap water
Pyrene	0.45	N/A	Mineral water
Quinoxifen	0.087	45 4.5	Tap water
Simazine	1.9	300 300	River water

Table 2 (cont.). Established LOQs for all analytes compared to required LOQs derived from 2013/39/EU, OGWV or Commission Implementing Decision (EU) 2015/495.

Analyte	LOQ [ng/L]	Required LOQ for „inland surface waters“ and „other surface waters“ [ng/L] ¹	Matrix
Terbutryne	0.10	19.5 1.95	Tap water
Triallate	0.084	670	Tap water
Tri-n-butyl phosphate	9.7	3000	River water
1,2,3-Trichlorobenzene	0.95	120 120	River water
1,2,4-Trichlorobenzene	1.2	120 120	River water
1,3,5-Trichlorobenzene	0.18	120 120	River water
Triclosan	1.4	N/A	Mineral water
Trifluralin	0.19	9 9	River water
Tris(2-chloroisopropyl) phosphate (TCPP)	29	N/A	Tap water

¹ Calculated as 0.3 x AA-EQS according to 2013/39/EU or 0.3 x EQS according to OGWV (July 20th 2011) or „Maximum acceptable method detection limit“ according to Commission Implementing Decision (EU) 2015/495

² AA-EQS refers to the sum of concentrations of the cyclodiene pesticides aldrin, dieldrin, endrin und isodrin. The required LOQ was calculated under the assumption that only one of the respective analytes is present in the sample (worst case scenario)

³ Calculated under consideration of MAC-EQS since no AA-EQS is defined

⁴ AA-EQS refers to the sum of concentrations of p,p'-DDT, o,p'-DDT, p,p'-DDE und p,p'-DDD. The required LOQ was calculated under the assumption that only one of the respective analytes is present in the sample (worst case scenario)

⁵ AA-EQS refers to the sum of concentrations of the isomers alpha- und beta-endosulfan. The required LOQ was calculated under the assumption that only one of the respective analytes is present in the sample (worst case scenario)

⁶ AA-EQS refers to the sum of concentrations of the isomers. The required LOQ was calculated under the assumption that only one of the respective isomers is present in the sample (worst case scenario)

⁷ AA-EQS refers to the sum of concentrations of the congeners 28, 47, 99, 100, 153 und 154. The required LOQ was calculated under the assumption that only one of the respective analytes is present in the sample (worst case scenario)

Table 3. Relative uncertainty of measurement for priority compounds listed in the EU-WFD near their respective EQS.

Analyte	Conc. [ng/L]	Uncertainty of measurement [%]
Aclonifen	9.9	23.2
Alachlor	52	16.0
Aldrin	3.3	15.1
Anthracene	2.5	17.9
Atrazine	14	23.2
Benzo[a]pyrene	0.10	27.3
Bifenox	2.1	29.7
Bis(2-ethyl-hexyl) phthalate (DEHP)	134	30.5
Chlorfenvinphos	20	45.3
Chlorpyrifos-ethyl	12	39.1
Cybutryne (Irgarol 1051)	0.75	44.0
Cypermethrin	0.20	35.6
p,p'-DDD	3.3	25.0
p,p'-DDE	3.3	29.3
o,p'-DDT	3.3	23.7
p,p'-DDT	3.3	17.0
Dichlorvos	0.29	22.7
Dicofol	0.15	16.3
Dieldrin	3.3	21.6
Endosulfan	0.59	18.6
Endrin	3.3	22.0
Fluoranthene	2.5	23.2
α-Hexachlorocyclohexane	1.3	24.2
β- Hexachlorocyclohexane	1.3	24.9
δ- Hexachlorocyclohexane	1.3	18.0
γ- Hexachlorocyclohexane	1.3	29.8

Analyte	Conc. [ng/L]	Uncertainty of measurement [%]
Heptachlor	0.052	33.2
Heptachlor-endo-epoxide	0.052	43.3
Hexachlorobenzene	6.5	30.0
Hexachlorobutadiene	37	25.1
Isodrin	3.7	19.0
Naphthalene	5.0	15.7
4-Nonylphenols	260	32.0
4-tert.-Octylphenol	13	37.9
PBDE 28	0.55	24.6
PBDE 47	0.28	20.0
PBDE 99	0.11	45.1
PBDE 100	0.55	13.4
PBDE 153	0.55	33.5
PBDE 154	0.28	20.9
Pentachlorobenzene	0.86	40.0
Pentachlorophenol	35	18.3
Quinoxifen	16	17.3
Simazine	29	20.1
Terbutryne	5.7	21.3
1,2,3-Trichlorobenzene	11	38.2
1,2,4-Trichlorobenzene	13	46.9
1,3,5-Trichlorobenzene	4.5	20.7
Trifluralin	4.7	24.4

Table 4. Analysis values for real world samples.

Compound / ng/L	Sewage treatment plant effluent, mid-west Germany	River, south-west Germany	Canal, mid-west Germany	River, mid-west Germany	Brook, low mountains, mid-west Germany	Tap water, mid-west Germany	Small river, Alps, Austria
Acenaphthene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Acenaphthylene	0.23	0.51	<LOQ	0.10	<LOQ	<LOQ	<LOQ
Aclonifen	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Alachlor	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Aldrin	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Ametryne	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Anthracene	0.44	1.0	0.28	0.21	0.13	<LOQ	<LOQ
Atrazine	1.9	2.2	0.51	0.98	2.2	<LOQ	<LOQ
Benz[a]anthracene	1.4	0.75	0.21	<LOQ	0.11	<LOQ	<LOQ
Benzo[a]pyrene	1.9	0.95	0.34	0.34	0.19	<LOQ	<LOQ
Benzo[b]fluoranthene	2.2	2.3	0.34	0.71	0.47	<LOQ	<LOQ
Benzo[g,h,i]perylene	2.0	1.0	0.20	0.30	0.13	<LOQ	<LOQ
Benzo[k]fluoranthene	1.1	1.2	0.21	0.28	0.38	<LOQ	<LOQ
Bifenox	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Biphenyl	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Bis-(2-ethylhexyl) phthalate (DEHP)	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
cis-Chlordane	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
trans-Chlordane	<LOQ	<LOQ	0.035	<LOQ	0.029	0.038	<LOQ
Chlorfenvinphos	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Chlorpyrifos-ethyl	0.23	0.056	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Chrysene	1.9	1.1	0.41	1.0	0.25	<LOQ	<LOQ
Cybutryne (Irgarol 1051)	0.28	0.39	1.1	0.29	<LOQ	<LOQ	<LOQ
Cypermethrin (4 isomers)	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
p,p'-DDD	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
p,p'-DDE	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
o,p'-DDT	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
p,p'-DDT	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Dibenz[a,h]anthracene	0.20	<LOQ	<LOQ	0.12	<LOQ	<LOQ	<LOQ
Dichlobenil	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Dichlorvos	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Dicofol	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Dieldrin	0.084	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Diflufenican	0.39	1.3	2.6	0.18	<LOQ	<LOQ	<LOQ
2,6-Di-tert-butyl-4-methylphenol	6.4	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
α -Endosulfan	0.13	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
β -Endosulfan	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Endosulfan sulfate	<LOQ	0.056	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Endrin	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Endrin ketone	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Ethofumesate	0.32	0.084	<LOQ	0.16	<LOQ	<LOQ	<LOQ
Fenitrothion	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Fenpropimorph	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ

Table 4 (cont.). Analysis values for real world samples.

Compound / ng/L	Sewage treatment plant effluent, mid-west Germany	River, south-west Germany	Canal, mid-west Germany	River, mid-west Germany	Brook, low mountains, mid-west Germany	Tap water, mid-west Germany	Small river, Alps, Austria
Fluoranthene	2.5	1.5	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Fluorene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Heptachlor	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Heptachlor-endo-epoxide	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Hexachlorobenzene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Hexachlorobutadiene	<LOQ	0.26	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
α -Hexachlorocyclohexane	0.070	0.15	0.14	<LOQ	0.060	0.065	<LOQ
β -Hexachlorocyclohexane	0.31	0.19	<LOQ	<LOQ	0.18	0.14	<LOQ
γ -Hexachlorocyclohexane	1.4	0.45	0.11	0.17	0.065	0.056	<LOQ
δ -Hexachlorocyclohexane	<LOQ	0.065	0.052	<LOQ	0.052	<LOQ	<LOQ
Indeno[1,2,3-cd]pyrene	2.6	1.5	0.39	0.33	0.15	<LOQ	<LOQ
Isodrin	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Methoxychlor	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Metolachlor	3.7	0.21	>4.8	0.52	0.076	0.086	<LOQ
Naphthalene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
4-Nonylphenols (tech. mixture)	199	19	11	21	<LOQ	<LOQ	<LOQ
4-tert.-Octylphenol	10	1.2	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Oxadiazon	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 28	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 47	0.097	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 99	0.23	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 100	0.048	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 153	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 154	0.027	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PBDE 183	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 77	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 81	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 105	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 114	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 118	0.033	<LOQ	0.021	<LOQ	<LOQ	<LOQ	<LOQ
PCB 123	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 126	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 156	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 157	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 167	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 169	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
PCB 189	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Pendimethalin	0.40	1.7	<LOQ	<LOQ	0.21	<LOQ	<LOQ
Pentachlorobenzene	0.096	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Pentachlorophenol	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Phenanthrene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Picolinafen	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Prometon	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ

Compound / ng/L	Sewage treatment plant effluent, mid-west Germany	River, south-west Germany	Canal, mid-west Germany	River, mid-west Germany	Brook, low mountains, mid-west Germany	Tap water, mid-west Germany	Small river, Alps, Austria
Prometryne	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Propazine	0.11	0.19	<LOQ	0.14	0.25	<LOQ	<LOQ
Propiconazole	6.1	5.8	0.48	2.6	>9.6	<LOQ	<LOQ
Propyzamide	2.9	5.4	19	0.79	<LOQ	<LOQ	<LOQ
Pyrene	<LOQ	2.1	0.49	<LOQ	<LOQ	<LOQ	<LOQ
Quinoxifen	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Simazine	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Terbutryne	6.8	13	0.25	5.1	0.92	<LOQ	<LOQ
Triallate	0.15	0.32	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
1,2,3-Trichlorobenzene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
1,2,4-Trichlorobenzene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
1,3,5-Trichlorobenzene	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Triclosan	9.9	3.8	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Trifluralin	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Tri-n-butyl phosphate	39	11	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ
Tris(2-chloroisopropyl) phosphate (TCPP)	>300	296	54	166	<LOQ	<LOQ	<LOQ

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