Application note | 003943

Environmental

# Automated liquid-liquid extraction workflow for direct ultra-trace analysis of pesticides and PAHs in water matrices using GC-MS/MS

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**Keywords**

Surface water, drinking water, polyaromatic hydrocarbons, PAH, pesticides, large volume injection, matrix facilitated degradation, TriPlus RSH SMART autosampler, liquid-liquid extraction (LLE), Sampling Workflow Editor software

## Goal

The goal of this application note is to demonstrate the capabilities of the Thermo Scientific™ TriPlus™ RSH SMART autosampler to perform automated sample preparation on-line with the analysis of semi-volatile organic compounds (SVOCs) in water at ultra-trace levels using large volume injection gas chromatography – triple quadrupole mass spectrometry.

## Introduction

Ensuring high standards of water quality is a fundamental priority within the European Union. This is highlighted through stringent EU regulations, such as the Water Framework Directive and the Drinking Water Directive,[1] where protection of the environment and safeguarding public health are of utmost importance. As such, regular monitoring of both surface and drinking water for hazardous semi-volatile organic compounds, such as polyaromatic hydrocarbons (PAHs) and pesticides, is needed.[1,2]

To meet regulatory compliance, laboratories are required to reach ultra-trace levels (i.e., parts per-trillion (ng/L)), while maintaining analytical method performance criteria outlined under EU Directive 2020/2184.[3] To reach required concentration limits, laboratories typically need to extract large sample volumes using solvent (i.e., liquid-liquid) or sorbent-based (i.e., solid-phase) extraction techniques with additional preconcentration.

Such techniques involve manual operations, which are costly in terms of consumables and time. However, automated sample preparation and extraction can reduce such costs while helping to eliminate systematic errors to improve data quality and lab efficiency.

The aim of this work was to evaluate the sensitivity, precision, and robustness of the TriPlus RSH SMART autosampler in performing automated liquid-liquid extraction and on-line analysis of polyaromatic hydrocarbons (PAHs) and pesticides in drinking and surface water using triple quadrupole GC-MS/MS. This study will demonstrate that the developed automated workflow is compliant with EU regulation criteria and greatly increases laboratory productivity by reducing laboratory costs and time.

## Experimental

### Standard and sample preparation

A native mixture of 18 individual PAH components—EPA Method 8270 standard (P/N 31995), labeled PAH internal standard (P/N 312206), and GC Multiresidue Pesticide Standard kit (P/N 32562)—were purchased from Restek. Labeled internal standards of ($D_6$)-alpha-HCH, ($D_{10}$)-diazinon, and ($D_8$)-o, p´-DDT together with triphenyl phosphate as a syringe standard were purchased from LGC standards. A stock solution of native PAH compounds and solution 2 (P/N 32564), solution 3 (P/N 32565), solution 6 (P/N 32568), and solution 7 (P/N 32569) from the GC Multiresidue Pesticide Standard kit was prepared at a concentration of 2 µg/mL in methanol. A full overview of targeted analytes can be found in the appendix (Table A1). From this primary stock solution, individual stock solutions of 4, 10, 20, 100, 200, and 300 ng/mL were prepared in methanol for calibration curve construction. Using a 10 µL gas tight syringe, a 5 µL aliquot from the respective individual stock solution was added into 10 mL of ultrapure water (18.2 MΩ) to produce the desired concentration. A 7-point calibration curve ranging from 2 to 150 ng/L was evaluated together with check standards (10 ng/L) to assess calibration validity over the analysis period. Drinking and surface water samples were spiked at 10 ng/L and 5 ng/L, respectively, to access extraction efficiency and precision of the automated workflow.

A labeled PAH/Pesticide internal standard mixture and syringe standard were prepared in methanol at concentrations of 100 ng/mL and 20 ng/mL, respectively. Drinking water and surface water were collected from the city of Bremen, Germany, for method validation. A 10 mL aliquot was pipetted into a 20 mL screw top headspace vial (P/N 6ASV20-1) prior to automated sample preparation and extraction.

### Instrument and method setup

A Thermo Scientific™ TRACE™ 1610 GC equipped with a Thermo Scientific™ TraceGOLD™ TG5-SilMS (30 m × 0.25 mm I.D. × 0.25 µm film) capillary column with a 5 m integrated SafeGuard retention gap (P/N 26096-1425) was used to perform the chromatographic separation. The TriPlus RSH SMART autosampler was configured to perform automated sample preparation, liquid-liquid extraction, and on-line injection for GC-MS/MS analysis. The automated workflow was designed using the Thermo Scientific™ TriPlus™ RSH Sampling Workflow Editor Software (P/N 1R77010-1200) and imported into the Thermo Scientific™ Chromeleon™ 7.3.2 Chromatography Data System (CDS) software. This integration allows sample preparation, acquisition, and data processing to be carried out within a single software. The automated workflow involved the following steps: internal standard addition, extraction solvent addition (pentane) and vortexing for extraction, addition of solvent for emulsion removal (isopropyl alcohol), addition of syringe standard prior to analysis, and large volume injection into the GC-MS. Parameter settings for the automated workflow are outlined in Table 1 with a visual overview provided in Figure 1. A list of accessories needed to configure the TriPlus RSH SMART autosampler is provided in the appendix (Table A2).

After sample extraction was completed, a 30 µL aliquot of the pentane layer was directly injected into a programmable temperature vaporization (PTV) inlet. Injection and oven program conditions can be found described in Tables 1 and 2. Data acquisition was carried out using selected reaction monitoring (SRM) with a Thermo Scientific™ TSQ™ 9610 triple quadrupole GC-MS equipped with an Advanced Electron Ionization (AEI) source. Method parameters for data acquisition are summarized in Table 2 with optimized SRM transitions outlined in the appendix (Table A3).

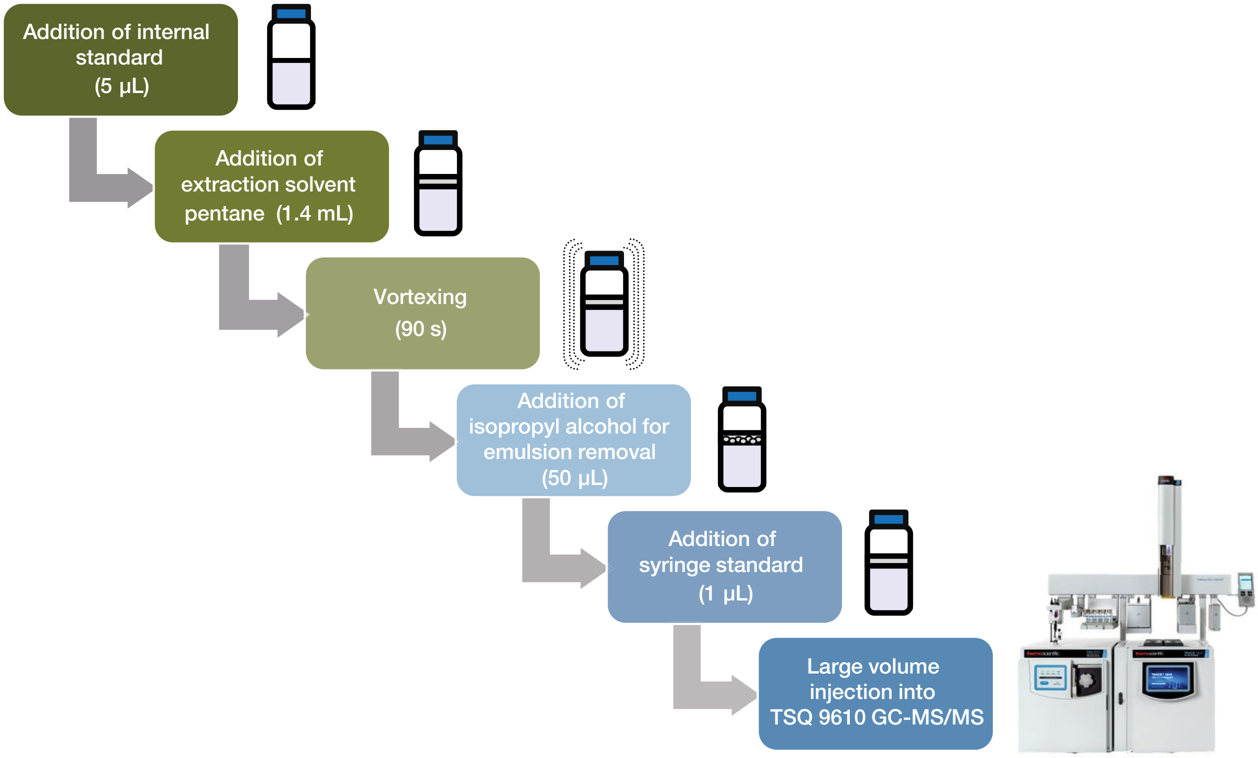

**Figure 1. Visual overview of automated workflow for sample preparation and liquid-liquid extraction of water samples by the TriPlus RSH SMART robotic autosampler**

**Table 1. TriPlus RSH SMART autosampler parameters**

| Workflow settings | | | |
|---|---|---|---|
| **Internal standard addition – 10 µL syringe** | | **Emulsion removal – 100 µL syringe** | |
| Aliquot volume (µL) | 5 | Solvent aliquot volume (isopropyl alcohol) (µL) | 50 |
| Fill speed (µL/s) | 1 | Wash cycles | 2 |
| Dispense speed (µL/s) | 20 | Wash syringe volume (%) | 70 |
| Syringe rinsing cycles | 1 | Fill speed (µL/s) | 10 |
| Sample rinsing volume (µL) | 5 | Dispense speed (µL/s) | 250 |
| Vial penetration depth (mm) | 31 | Sample vial penetration depth (mm) | 40 |
| Syringe post-solvent volume (acetone) | 70% | **Syringe standard addition – 10 µL syringe** | |
| Syringe post-solvent cycles (acetone) | 2 | Aliquot volume (µL) | 1 |
| **Extraction solvent addition – 1,000 µL syringe** | | Wash cycles | 3 |
| Solvent aliquot volume (pentane) (µL) | 1,400 (2 × 700 µL) | Wash syringe volume (%) | 70 |
| Fill speed (µL/s) | 20 | Fill speed (µL/s) | 1 |
| Dispense speed (µL/s) | 300 | Dispense speed (µL/s) | 20 |
| Vortexer speed (rpm) | 1,990 | Sample vial penetration depth (mm) | 31 |
| Vortexer time (s) | 90 | **Sample injection – 100 µL syringe** | |
| | | Sample volume | 30 |
| | | Wash steps (pentane) | 3 |
| | | Wash syringe volume (%) | 50 |
| | | Fill speed (µL/s) | 2 |
| | | Sample vial penetration (mm) | 42.5 |
| | | Injection speed (µL/s) | 3 |
| | | Injector penetration depth (mm) | 40 |

Table 2. GC-MS/MS operation conditions

| **Injector conditions** | | | | |
|---|---|---|---|---|
| Injector | Thermo Scientific™ iConnect™ PTV | | | |
| Liner | Thermo Scientific™ sintered PTV liner with concentric baffle (P/N 45352060) | | | |
| Injection volume (µL) | 30 | | | |
| Inlet temperature (°C) | 40 | | | |
| Carrier gas flow (mL·min$^{-1}$) | 1.2 | | | |
| Injection type | Large volume | | | |
| Splitless time (min) | 2.0 | | | |
| Split flow (mL·min$^{-1}$) | 50 | | | |
| Injection vial depth (mm) | 42.5 | | | |
| **PTV ramp settings** | **Rate (°C·s$^{-1}$)** | **Temp (°C)** | **Time (min)** | **Flow (mL·min$^{-1}$)** |
| Injection phase | - | - | 0.1 | 20 |
| Transfer phase | 14.5 | 320 | 2.0 | - |
| Cleaning phase | 14.5 | 330 | 5.0 | 75 |
| **Oven temperature program** | | | | |
| Initial temperature (°C) | 50 | | | |
| Hold time (min) | 2 | | | |
| Rate 1 (°C·min$^{-1}$) | 25 | | | |
| Temperature 1 (°C) | 150 | | | |
| Rate 2 (°C·min$^{-1}$) | 8.93 | | | |
| Temperature 2 (°C) | 175 | | | |
| Rate 3 (°C·min$^{-1}$) | 5.18 | | | |
| Temperature 3 (°C) | 320 | | | |
| Final temperature hold time (min) | 5 | | | |
| Total analysis time (min) | 41.8 | | | |
| **TSQ 9610 mass spectrometer conditions** | | | | |
| Transfer line (°C) | 300 | | | |
| AEI Ion source temperature (°C) | 320 | | | |
| Electron energy (eV) | 50 | | | |
| Acquisition mode | Timed-SRM | | | |
| Emission current (µA) | 10 | | | |
| Collision gas and pressure (psi) | Argon, 70 | | | |

## Results and discussion

### Calibration and sensitivity performance

A total of 78 compounds were targeted in this analysis (Appendix Table A1). All compounds showed linear correlation with coefficient of determination ($r^2$) > 0.99 over the entire calibration range (2–150 ng/L). Representative examples for different substance classes under investigation are displayed in Figure 2. A complete overview of calibration responses for all analytes is provided in appendix (Table A1).

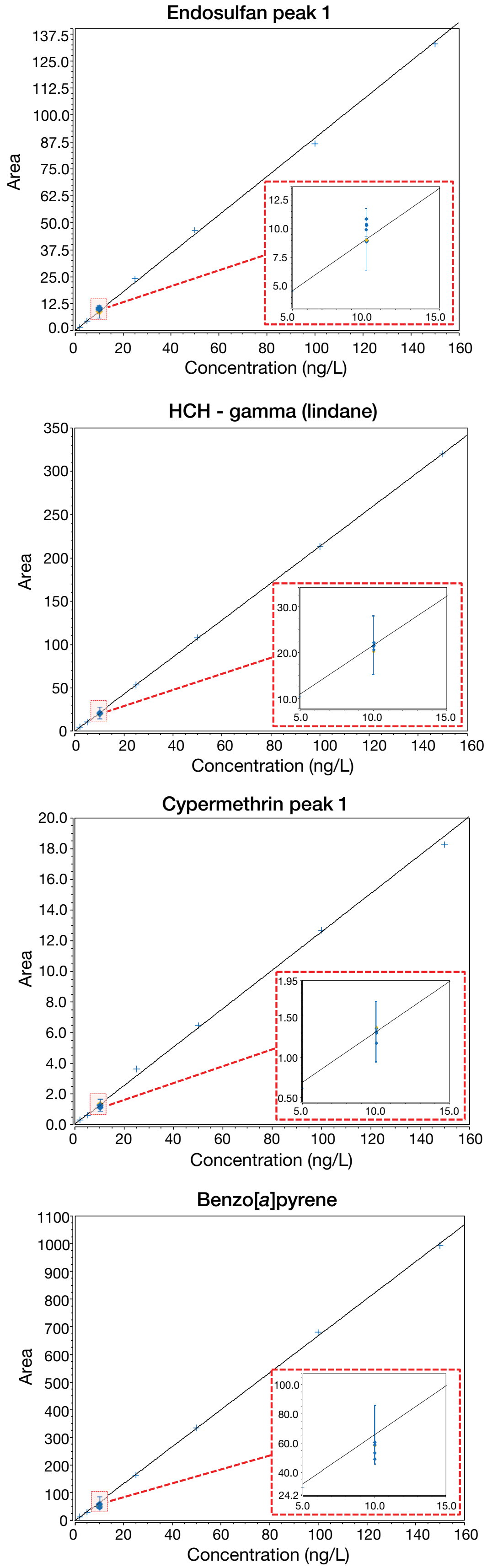

**Figure 2. Calibration curves (2–150 ng/L) for endosulfan peak 1, hexachlorocyclohexane – gamma (lindane), cypermethrin peak 1, and benzo[*a*]pyrene.** The highlighted region shows the results of the individual quality check (QC) standards (10 ng/L) and the 30% precision threshold to the calibration response.

Detection and quantification limits were determined based on the analytical variation observed in replicate analyses of the lowest calibration standard (i.e., 2 ng/L). After 8 replicate injections, the standard deviation was multiplied by a factor of 3 and 10 to determine the limits of detection (LOD) and quantification (LOQ), respectively (Appendix Table A4). Criteria under EU Directive 2020/2184 specify LOQ values must be at least 30% of the environmental quality standard specified for benzo[*a*]pyrene (10 ng/L; LOQ ≤ 3 ng/L), sum PAH (defined as sum of benzo[*b*]-fluoranthene, benzo[*k*]fluoranthene, benzo[*g,h,i*]perylene, indeno[1,2,3-*cd*]pyrene) (100 ng/L; LOQ ≤ 30 ng/L), and pesticides (100 ng/L; LOQ ≤ 30 ng/L). Limits of quantification obtained using the automated extraction workflow for benzo[*a*]pyrene (2.9 ng/L), sum PAHs (1.46–2.42 ng/L), and targeted pesticides (0.38–9.35 ng/L) were within the specified criteria. In addition, 72% of the 78 targeted compounds had LOQs less than 2 ng/L, demonstrating method compliance towards sensitivity requirements.

## Extraction recovery performance

Method performance towards extraction recovery was assessed through the spike and recovery experiments. Surface and drinking water samples were spiked at 5 and 10 ng/L, respectively, followed by analysis using the automated workflow. Three separate replicates of spiked samples were prepared, with results of these experiments shown in Figures 3 and 4.

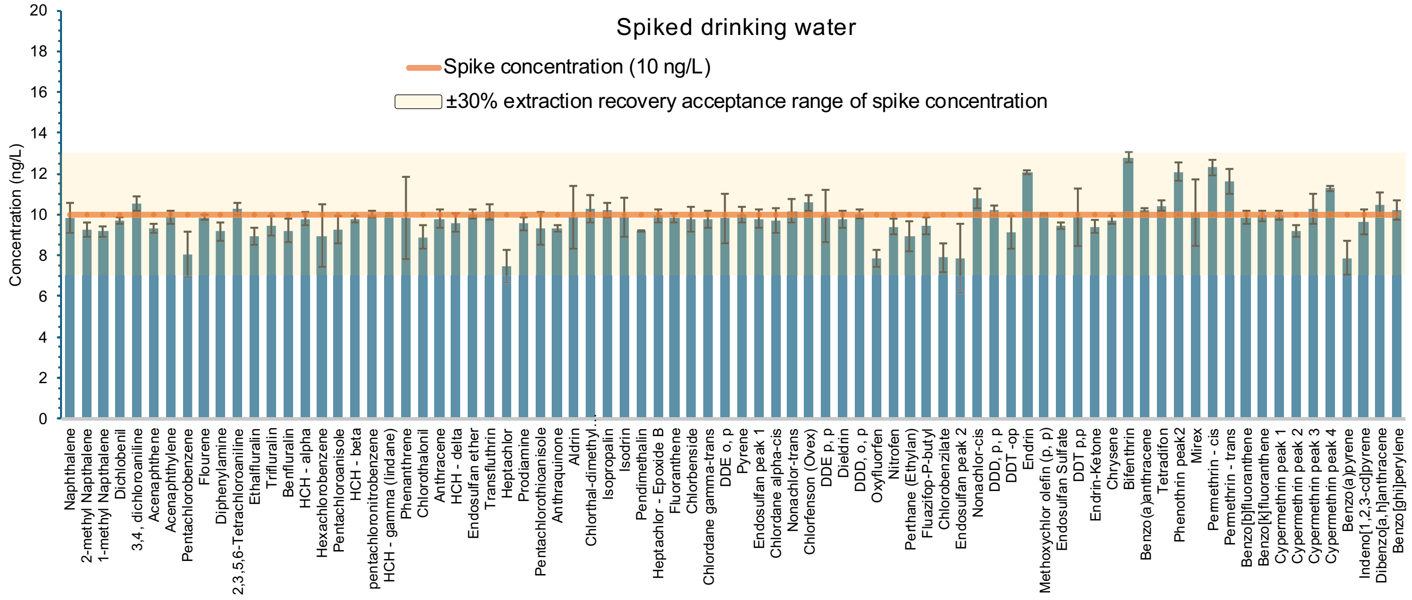

**Figure 3. Results of the extraction recovery experiment for spiked drinking water at 10 ng/L.** The shaded region represents the ±30% extraction recovery acceptance range (i.e., 70–130%) of the spiked concentration.

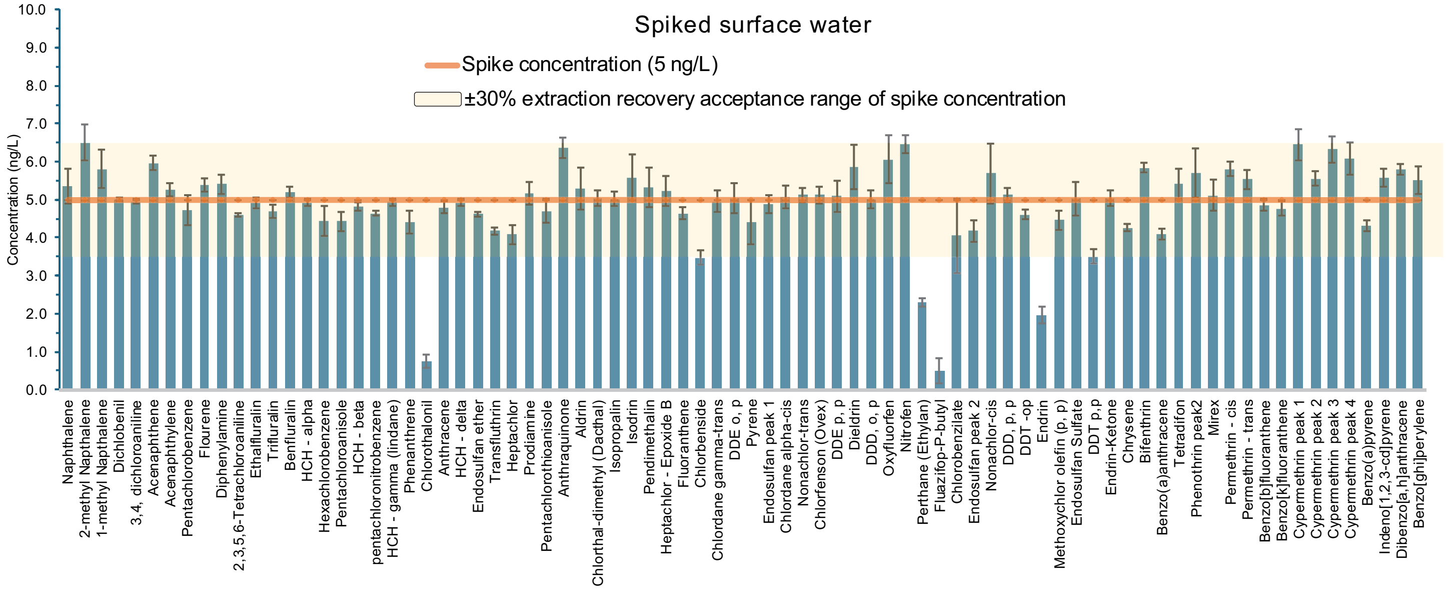

**Figure 4. Results of extraction recovery experiment for spiked surface water at 5 ng/L.** The shaded region represents the ±30% extraction recovery acceptance range (i.e., 70–130%) of the spiked concentration.

Most validated methods require extraction recoveries to be within 70–130%. In spiked drinking water, this criterion is achieved with extraction recoveries for all analytes being within ±30% of the spiked concentration (Figure 3). Similar results were observed in spiked surface water experiments at the lower spike concentration of 5 ng/L. However, several compounds showed extraction recoveries outside the ±30% recovery range (i.e., chlorothalonil, chlorobenside, perthane (Ethylan™), fluazifop-p-butyl, endrin, and p,p´-DDT) (Figure 4). Although surface water experiments employed a lower spike concentration (5 ng/L) compared to drinking water experiments (10 ng/L), these results may indicate possible matrix associated degradation within surface water. To test this hypothesis, surface water was spiked at 10 ng/L and processed again using the automated workflow. At 10 ng/L spike concentration, recovery of chlorothalonil, chlorbenside, fluazifop-p-butyl, and endrin still fell below the acceptable extraction recovery range (Figure 5).

Extraction recoveries of these analytes were significantly lower compared to results obtained in drinking water, indicating matrix facilitated degradation. The range of degradation is also not consistent across all compounds, indicating differences in compound specific degradation rates. Addition of isotopic-labeled standards for these compounds can correct for compound specific degradation, improving data accuracy for the analysis of these compounds in surface waters.

## Method precision and robustness

To evaluate the robustness of the automated workflow, a sequence of 80 drinking water samples (65-hour total analysis time) was carried out with periodic analysis of 10 ng/L quality control standards (n = 6) (Figure 6).

Method precision requirements specified under EU Directive 2020/2184 require the method precision of PAHs and pesticides when measured at the specified environmental quality standard level (i.e., 100 ng/L) be within ±40% and ±30%, respectively. Although our QC standard concentrations were a factor of 10 lower than the environmental quality standard level, all PAHs were within the specified method precision criteria across all QC samples. Similar results were observed for pesticides, with exception to QC2 where heptachlor and mirex fell outside the specified range. However, under EU Directive 2020/2184, a higher uncertainty “may be allowed for a number of pesticides” considering the wide range in chemistry this class of chemicals possesses. All remaining QC standards were within the ±30% of the spiked concentration, demonstrating the robust performance in method precision for the automated liquid-liquid extraction workflow.

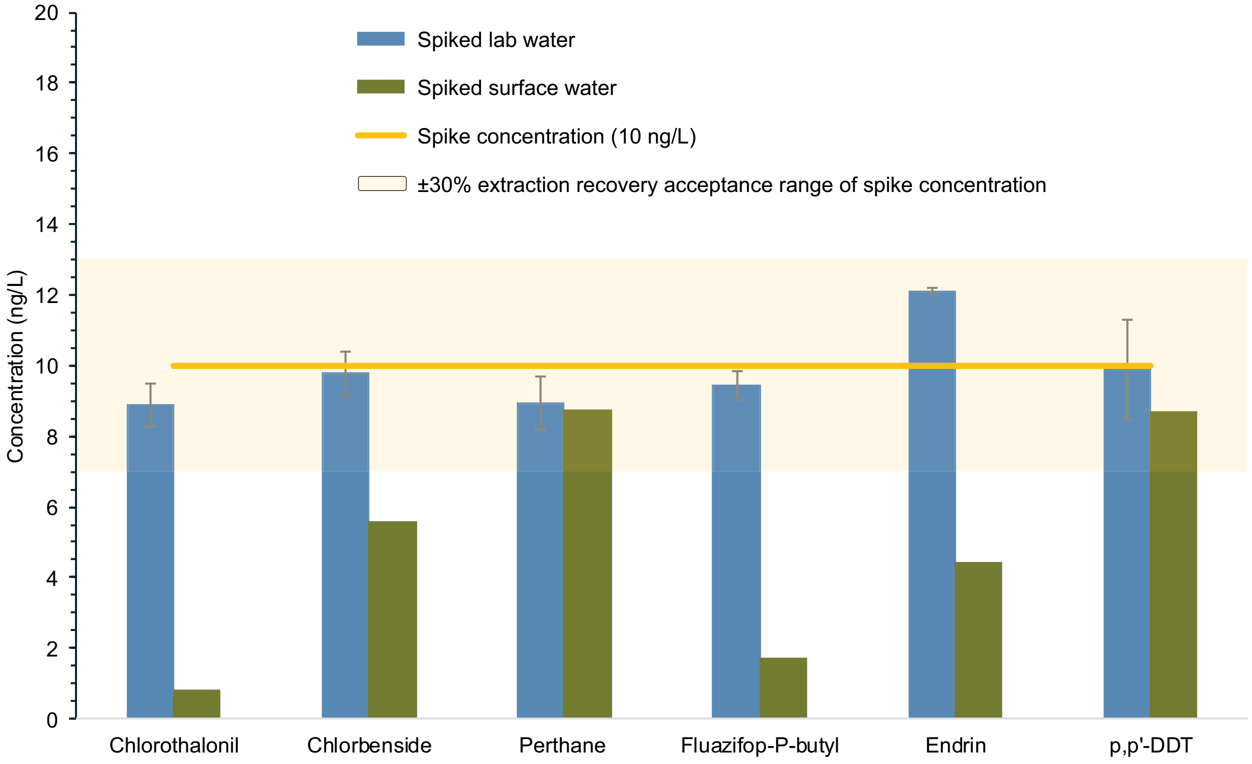

**Figure 5. Extraction recovery comparison between drinking water and surface water spiked at 10 ng/L.** The shaded region represents ±30% extraction recovery acceptance range (i.e., 70–130%) of spiked concentration.

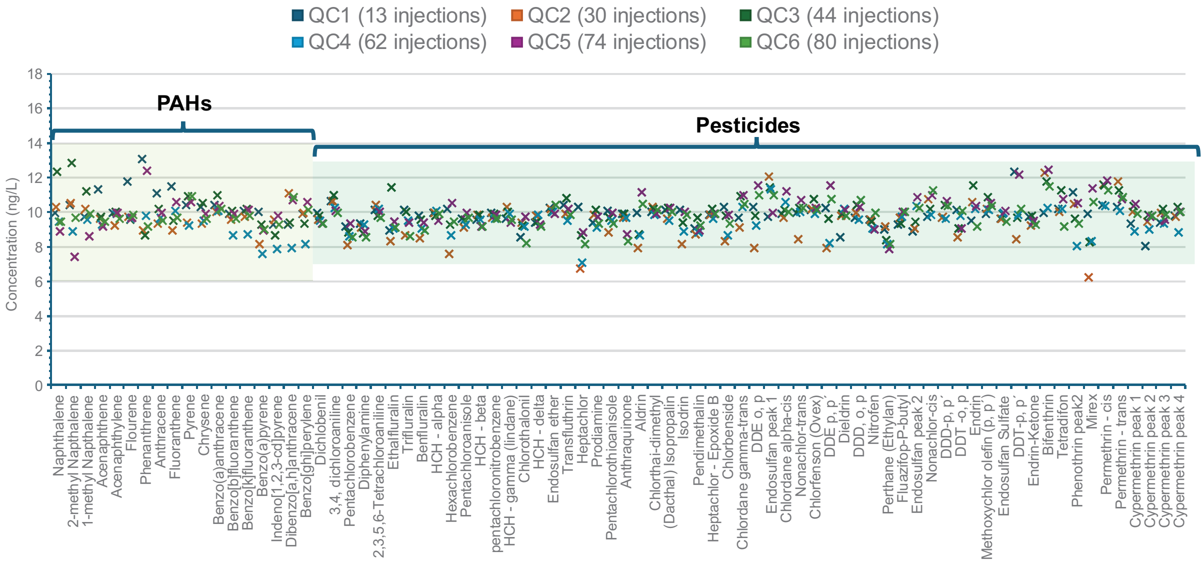

**Figure 6. Method precision of quality control (QC) standard (10 ng/L) after 80 sample injections.** Results of each QC standard result are displayed for each analyte. The shaded region represents the method precision criteria for PAHs (±40%) and pesticides (±30%) specified under EU Directive 2020/2184.

## Benefits of automated LLE extraction workflow

Solvent extraction is a long-standing "gold standard" for isolating organic pollutants like PAHs and pesticides from water. However, traditional separatory-funnel liquid-liquid extraction is laborious, time-consuming, error-prone, and requires large amounts of sample and solvent. Using manual preparation, 200 mL of solvent is required for a single water sample. For the robustness experiment carried out above, 16 L of solvent would be required to extract 80 samples. With the automated workflow, we can achieve the same throughput with only 120 mL of solvent.

Achieving ultra-trace limits as required by the EU Directive 2020/2184 while processing many samples demands robust, high-throughput workflows that can be achieved only by automating manual steps. Automated sample preparation workflows executed by the TriPlus RSH SMART robotic autosampler address this need by streamlining routine extraction protocols and enforcing strict, repeatable procedures. Automation turns an LLE procedure into a hands-off, unattended process—dramatically improving precision, speed, safety, and data integrity compared to manual extraction, freeing skilled analysts from tedious hands-on work.[4]

### Key benefits can be summarized as follows:

- Operational efficiency and throughput, thanks to unattended 24/7 operation
- Waste reduction since a limited volume of solvent is required
- Confidence in quantitative results due to higher precision and accuracy of error-free robotic operation
- Method compliance and traceability in Chromeleon CDS

## Conclusions

Maintaining water quality is of both human and environmental health importance. However, due to the physical chemical properties of various organic substances, analytical methods require ultra-trace sensitivity and accuracy to quantify hazardous risks within both drinking and environmental surface waters. The results presented demonstrate that the developed automated workflow for online liquid-liquid extraction and analysis of water samples can meet these requirements:

- Ultra-trace sensitivity combining large volume injection with highly sensitive triple quadrupole GC-MS/MS, with over 70% of targeted analytes having limits of quantification below 2 ng/L
- Compliant extraction recovery at part per trillion concentrations
- Robust method precision over extended analysis time
- Improved laboratory efficiency and productivity while reducing environmental impact with limited solvent consumption
- Workflow customization capability through the Sampling Workflow Editor software

### References

1. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000: Establishing a framework for Community action in the field of water policy. https://eur-lex.europa.eu/eli/dir/2000/60/oj
2. European Council Directive 98/83/EC of 3 November 1998: On the quality of water intended for human consumption. https://eur-lex.europa.eu/eli/dir/1998/83/oj/
3. Directive (EU) 2020/2184 of the European Parliament and of the Council of 16 December 2020: On the quality of water intended for human consumption (recast). https://eur-lex.europa.eu/eli/dir/2020/2184/oj/
4. Thermo Fisher Scientific Case Study 001327 - VERITAS meets increasing sample analysis demands, saves time, and minimizes costs with the TriPlus Robotic Sample Handling (RSH) autosampler
5. Thermo Fisher Scientific - Automated Workflow Solutions for GC and GC-MS

## Appendix

**Table A1. Targeted analytes list with chromatographic retention time, relative standard deviation of calibration response, and coefficient of determination for linear response**

| Peak name | Ret. time (min) | Rel. std. dev. (%) | Coeff. of determination |
|---|---|---|---|
| Naphthalene | 6.76 | 1.19 | 0.9996 |
| 2-methyl Napthalene | 7.62 | 1.96 | 0.9973 |
| 1-methyl Napthalene | 7.75 | 1.97 | 0.9991 |
| Dichlobenil | 7.91 | 4.79 | 0.9997 |
| 3,4, Dichloroaniline | 8.68 | 5.47 | 0.9996 |
| Acenaphthylene | 8.99 | 4.46 | 0.9997 |
| Acenaphthene | 9.3 | 2.33 | 0.9999 |
| Pentachlorobenzene | 9.58 | 9.25 | 0.9989 |
| Fluorene | 10.37 | 4.46 | 0.9996 |
| Diphenylamine | 10.67 | 4.94 | 0.9991 |
| 2,3,5,6-Tetrachloroaniline | 10.72 | 2.87 | 0.9999 |
| Ethalfluralin | 10.85 | 10.0 | 0.9988 |
| Trifluralin | 11.04 | 5.98 | 0.9996 |
| Benfluralin | 11.11 | 12.1 | 0.9982 |
| HCH - alpha | 11.62 | 3.33 | 0.9998 |
| Hexachlorobenzene | 11.76 | 8.06 | 0.9991 |
| Pentachloroanisole | 11.88 | 2.51 | 0.9999 |
| HCH - beta | 12.21 | 2.71 | 0.9999 |
| HCH - gamma (lindane) | 12.47 | 0.62 | 1.0000 |
| Pentachloronitrobenzene | 12.47 | 3.60 | 0.9998 |
| Phenanthrene | 12.89 | 9.37 | 0.9969 |
| Chlorothalonil | 12.91 | 9.62 | 0.9988 |
| Anthracene | 13.05 | 6.16 | 0.9994 |
| HCH - delta | 13.16 | 4.32 | 0.9997 |
| Endosulfan ether | 13.73 | 5.79 | 0.9995 |
| Transfluthrin | 14.35 | 7.06 | 0.9992 |
| Heptachlor | 14.52 | 7.89 | 0.9990 |
| Prodiamine | 14.98 | 4.86 | 0.9997 |
| Pentachlorothioanisole | 15.14 | 4.01 | 0.9998 |
| Aldrin | 15.59 | 9.80 | 0.9987 |
| Anthraquinone | 15.59 | 6.92 | 0.9992 |
| Chlorthal-dimethyl (Dacthal™) | 15.64 | 2.87 | 0.9999 |
| Isopropalin | 16.31 | 11.0 | 0.9983 |
| Isodrin | 16.48 | 6.80 | 0.9994 |
| Pendimethalin | 16.5 | 6.04 | 0.9995 |
| Heptachlor - Epoxide B | 16.79 | 6.56 | 0.9994 |
| Fluoranthene | 17.02 | 9.41 | 0.9982 |
| Chlorbenside | 17.48 | 7.75 | 0.9992 |
| Chlordane gamma-*trans* | 17.53 | 6.41 | 0.9994 |
| DDE o, p | 17.62 | 5.83 | 0.9995 |
| Pyrene | 17.86 | 4.76 | 0.9990 |
| Endosulfan peak 1 | 17.95 | 9.12 | 0.9988 |
| Chlordane alpha-*cis* | 17.95 | 14.2 | 0.9968 |
| Nonachlor-*trans* | 18.07 | 6.76 | 0.9993 |
| Chlorfenson (Ovex™) | 18.27 | 2.27 | 0.9999 |
| DDE p, p | 18.68 | 8.20 | 0.9990 |
| Dieldrin | 18.82 | 8.02 | 0.9988 |
| DDD, o, p | 18.89 | 10.9 | 0.9980 |
| Nitrofen | 19.44 | 10.0 | 0.9989 |
| Perthane (Ethylan) | 19.52 | 15.6 | 0.9956 |
| Fluazifop-p-butyl | 19.53 | 14.4 | 0.9966 |
| Endosulfan peak 2 | 19.83 | 12.6 | 0.9972 |
| DDD, p, p | 20.04 | 9.06 | 0.9987 |
| Nonachlor-*cis* | 20.05 | 12.9 | 0.9974 |
| DDT -op | 20.14 | 9.35 | 0.9988 |
| Endrin | 20.32 | 12.3 | 0.9972 |
| Methoxychlor olefin (p, p) | 20.95 | 7.54 | 0.9991 |
| Endosulfan sulfate | 21.11 | 9.40 | 0.9985 |
| DDT p,p | 21.31 | 14.8 | 0.9955 |
| Endrin-ketone | 22.65 | 8.94 | 0.9987 |
| Chrysene | 22.91 | 6.54 | 0.9994 |
| Bifenthrin | 23.02 | 16.8 | 0.9952 |
| Benz[*a*]anthracene | 23.05 | 4.77 | 0.9997 |
| Tetradifon | 23.87 | 8.87 | 0.9987 |
| Phenothrin peak 2 | 24.03 | 14.3 | 0.9937 |
| Mirex | 24.78 | 14.6 | 0.9968 |
| Permethrin - *cis* | 26.27 | 13.8 | 0.9969 |
| Permethrin - *trans* | 26.52 | 10.5 | 0.9976 |
| Benzo[*b*]fluoranthene | 27.32 | 3.49 | 0.9998 |
| Benzo[*k*]fluoranthene | 27.43 | 6.04 | 0.9995 |
| Cypermethrin peak 1 | 27.9 | 13.5 | 0.9971 |
| Cypermethrin peak 2 | 28.1 | 12.8 | 0.9971 |
| Cypermethrin peak 3 | 28.2 | 10.5 | 0.9982 |
| Cypermethrin peak 4 | 28.28 | 9.91 | 0.9984 |
| Benzo[*a*]pyrene | 28.51 | 6.06 | 0.9995 |
| Indeno[1,2,3-*cd*]pyrene | 32.43 | 9.98 | 0.9980 |
| Dibenzo[*a,h*]anthracene | 32.59 | 9.76 | 0.9981 |
| Benzo[*ghi*]perylene | 33.23 | 10.2 | 0.9979 |

**Table A2. TriPlus RSH SMART configuration and consumables**

| TriPlus RSH SMART configuration | Part number |
|---|---|
| TriPlus RSH SMART Advanced Autosampler for liquid injection, regular rail length | 1R77010-2003 |
| Automatic Tool Change Station | 1R77010-1019 |
| Liquid Syringe Tool for 57 mm syringe needle (0.5–100 µL syringe volume) | 1R77010-1007 |
| Liquid Syringe Tool for 57 mm syringe needle (250–1,000 µL syringe volume) | 1R77010-1009 |
| Solvent Station with 3 × 100 mL bottles | 1R77010-1031 |
| Vortexer | 1R77010-1033 |
| **Consumables** | |
| 10 µL Fixed Needle Gas-Tight SMART Syringe 23s Gauge 57 mm length | 365D0311SM |
| 100 µL Fixed Needle Gas-Tight SMART Syringe 26s Gauge 57 mm length with side hole | 365H2181-SM |
| 1,000 µL Fixed Needle Gas-Tight Syringe 22 Gauge 57 mm length | 365K2811-SM |
| Headspace Vial Cap, silver magnetic screw (18 mm) with silicone (blue)/PTFE seal | 6PMSC18-ST2 |
| Vial, 2 mL Amber Screw Glass (9 mm short thread), 100/pack | 6ASV9-2P |
| Headspace Vial, 20 mL clear screw glass, 100/pack | 6ASV20-1 |
| **Software** | |
| Sampling Workflow Editor software | 1R77010-1200 |

**Table A3 (Part 1). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS**

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Naphthalene D8 | 6.75 | 0.5 | 136 | 134.1 | 25 |
| Naphthalene D8 | 6.75 | 0.5 | 136 | 108 | 25 |
| Naphthalene | 6.77 | 0.5 | 128 | 78 | 25 |
| Naphthalene | 6.77 | 0.5 | 128 | 102 | 20 |
| Naphthalene | 6.77 | 0.5 | 128 | 126.9 | 16 |
| 2-methyl Napthalene | 7.61 | 0.5 | 141.1 | 115.1 | 16 |
| 2-methyl Napthalene | 7.61 | 0.5 | 142.1 | 115.1 | 26 |
| 2-methyl Napthalene | 7.61 | 0.5 | 142.1 | 141.1 | 14 |
| 1-methyl Napthalene | 7.74 | 0.5 | 141.1 | 115.1 | 16 |
| 1-methyl Napthalene | 7.74 | 0.5 | 142.1 | 115.1 | 26 |
| 1-methyl Napthalene | 7.74 | 0.5 | 142.1 | 141.1 | 14 |
| Dichlobenil | 7.91 | 0.5 | 170.9 | 99.9 | 24 |
| Dichlobenil | 7.91 | 0.5 | 170.9 | 136 | 12 |
| Dichlobenil | 7.91 | 0.5 | 172.8 | 99.8 | 24 |
| 3,4, Dichloroaniline | 8.69 | 0.5 | 160.9 | 99 | 20 |
| 3,4, Dichloroaniline | 8.69 | 0.5 | 160.9 | 90 | 18 |
| 3,4, Dichloroaniline | 8.69 | 0.5 | 160.9 | 126 | 10 |
| Acenaphthylene | 8.98 | 0.5 | 152 | 101.9 | 26 |
| Acenaphthylene | 8.98 | 0.5 | 152 | 150 | 28 |
| Acenaphthylene | 8.98 | 0.5 | 152 | 125.9 | 24 |
| Acenaphthene D10 | 9.24 | 0.5 | 162 | 160 | 20 |
| Acenaphthene D10 | 9.24 | 0.5 | 164 | 162 | 15 |
| Acenaphthene | 9.3 | 0.5 | 153 | 152 | 18 |
| Acenaphthene | 9.3 | 0.5 | 154 | 153 | 16 |
| Acenaphthene | 9.3 | 0.5 | 154 | 152 | 24 |
| Pentachlorobenzene | 9.58 | 0.5 | 249.8 | 214.8 | 16 |
| Pentachlorobenzene | 9.58 | 0.5 | 249.8 | 143.6 | 38 |
| Pentachlorobenzene | 9.58 | 0.5 | 249.8 | 178.5 | 24 |

**Table A3 (Part 2). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS**

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Fluorene | 10.36 | 0.5 | 165 | 164 | 16 |
| Fluorene | 10.36 | 0.5 | 166 | 115 | 38 |
| Fluorene | 10.36 | 0.5 | 165 | 163 | 30 |
| Diphenylamine | 10.67 | 0.5 | 168.1 | 167.1 | 14 |
| Diphenylamine | 10.67 | 0.5 | 169.2 | 167.1 | 22 |
| Diphenylamine | 10.67 | 0.5 | 168.1 | 139 | 38 |
| 2,3,5,6-Tetrachloroaniline | 10.73 | 0.5 | 230.8 | 157.9 | 18 |
| 2,3,5,6-Tetrachloroaniline | 10.73 | 0.5 | 230.8 | 159.8 | 18 |
| 2,3,5,6-Tetrachloroaniline | 10.73 | 0.5 | 230.8 | 194.8 | 10 |
| Ethalfluralin | 10.86 | 0.5 | 276 | 248.1 | 8 |
| Ethalfluralin | 10.86 | 0.5 | 315.9 | 276.1 | 8 |
| Ethalfluralin | 10.86 | 0.5 | 276 | 202 | 14 |
| Trifluralin | 11.05 | 0.5 | 306.1 | 264.1 | 8 |
| Trifluralin | 11.05 | 0.5 | 306.1 | 206 | 10 |
| Trifluralin | 11.05 | 0.5 | 306.1 | 159.7 | 20 |
| Benfluralin | 11.12 | 0.5 | 292 | 264 | 8 |
| Benfluralin | 11.12 | 0.5 | 292 | 159.7 | 20 |
| Benfluralin | 11.12 | 0.5 | 292 | 206.1 | 10 |
| aHCH-D6 | 11.52 | 0.5 | 221.9 | 185 | 8 |
| aHCH-D6 | 11.52 | 0.5 | 223.9 | 186.9 | 8 |
| HCH - alpha | 11.62 | 0.5 | 218.8 | 183 | 8 |
| HCH - alpha | 11.62 | 0.5 | 182.8 | 146.7 | 12 |
| Hexachlorobenzene | 11.76 | 0.5 | 283.8 | 248.8 | 18 |
| Hexachlorobenzene | 11.76 | 0.5 | 283.8 | 213.8 | 30 |
| Pentachloroanisole | 11.88 | 0.5 | 264.8 | 236.9 | 10 |
| Pentachloroanisole | 11.88 | 0.5 | 266.8 | 238.9 | 10 |
| Pentachloroanisole | 11.88 | 0.5 | 279.9 | 236.8 | 22 |
| HCH - beta | 12.21 | 0.5 | 180.9 | 145 | 14 |
| HCH - beta | 12.21 | 0.5 | 218.7 | 183 | 8 |
| HCH - gamma (lindane) | 12.46 | 0.5 | 180.9 | 145 | 14 |
| HCH - gamma (lindane) | 12.46 | 0.5 | 180.9 | 109 | 26 |
| Pentachloronitrobenzene | 12.47 | 0.5 | 274.8 | 239.9 | 18 |
| Pentachloronitrobenzene | 12.47 | 0.5 | 272.9 | 237.9 | 16 |
| Pentachloronitrobenzene | 12.47 | 0.5 | 274.8 | 204.9 | 28 |
| Diazinon D10 | 12.61 | 0.5 | 138.1 | 85.1 | 12 |
| Diazinon D10 | 12.61 | 0.5 | 200 | 135.1 | 8 |
| Fluchloralin | 12.78 | 0.5 | 306 | 264 | 8 |
| Fluchloralin | 12.78 | 0.5 | 264 | 159.5 | 14 |
| Fluchloralin | 12.78 | 0.5 | 264 | 206.1 | 8 |
| Phenanthrene D10 | 12.82 | 0.5 | 188 | 160 | 20 |
| Phenanthrene D10 | 12.82 | 0.5 | 188 | 184.1 | 28 |
| Phenanthrene | 12.9 | 0.5 | 178 | 152 | 20 |
| Phenanthrene | 12.9 | 0.5 | 178 | 151 | 32 |
| Phenanthrene | 12.9 | 0.5 | 178 | 176 | 35 |
| Chlorothalonil | 12.92 | 0.5 | 265.8 | 133 | 36 |
| Chlorothalonil | 12.92 | 0.5 | 228.8 | 168 | 8 |
| Chlorothalonil | 12.92 | 0.5 | 265.8 | 170 | 24 |

**Table A3 (Part 3). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS**

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Anthracene | 13.05 | 0.5 | 178 | 152 | 25 |
| Anthracene | 13.05 | 0.5 | 178 | 176 | 35 |
| Anthracene | 13.05 | 0.5 | 178 | 152 | 20 |
| Anthracene | 13.05 | 0.5 | 178 | 151 | 32 |
| HCH - delta | 13.16 | 0.5 | 218.8 | 182.9 | 8 |
| HCH - delta | 13.16 | 0.5 | 218.8 | 146.5 | 20 |
| Endosulfan ether | 13.72 | 0.5 | 69 | 41.1 | 12 |
| Endosulfan ether | 13.72 | 0.5 | 238.9 | 204 | 12 |
| Endosulfan ether | 13.72 | 0.5 | 240.9 | 206 | 14 |
| Chlozolinate | 14.02 | 0.5 | 259 | 187.9 | 12 |
| Chlozolinate | 14.02 | 0.5 | 259 | 152.9 | 26 |
| Chlozolinate | 14.02 | 0.5 | 331 | 259 | 8 |
| Transfluthrin | 14.35 | 0.5 | 163 | 143 | 14 |
| Transfluthrin | 14.35 | 0.5 | 127 | 91.1 | 8 |
| Transfluthrin | 14.35 | 0.5 | 163 | 91.1 | 12 |
| Metalaxyl | 14.47 | 0.5 | 131.9 | 117 | 12 |
| Metalaxyl | 14.47 | 0.5 | 160.1 | 130 | 18 |
| Metalaxyl | 14.47 | 0.5 | 160.1 | 144.8 | 10 |
| Heptachlor | 14.53 | 0.5 | 271.8 | 236.9 | 12 |
| Heptachlor | 14.53 | 0.5 | 99.8 | 65 | 12 |
| Heptachlor | 14.53 | 0.5 | 269.9 | 234.9 | 15 |
| Heptachlor | 14.53 | 0.5 | 271.9 | 236.9 | 15 |
| Prodiamine | 14.97 | 0.5 | 321.1 | 279.1 | 6 |
| Prodiamine | 14.97 | 0.5 | 275.1 | 255.1 | 8 |
| Prodiamine | 14.97 | 0.5 | 279 | 203.1 | 6 |
| Pentachlorothioanisole | 15.15 | 0.5 | 295.7 | 262.9 | 12 |
| Pentachlorothioanisole | 15.15 | 0.5 | 262.7 | 192.9 | 28 |
| Pentachlorothioanisole | 15.15 | 0.5 | 295.7 | 245.9 | 30 |
| Aldrin | 15.6 | 0.5 | 262.7 | 192.9 | 32 |
| Aldrin | 15.6 | 0.5 | 254.9 | 219.9 | 20 |
| Aldrin | 15.6 | 0.5 | 262.7 | 191 | 30 |
| Aldrin | 15.6 | 0.5 | 292.9 | 185.9 | 30 |
| Chlorthal-dimethyl (Dacthal) | 15.63 | 0.5 | 300.7 | 222.9 | 22 |
| Chlorthal-dimethyl (Dacthal) | 15.63 | 0.5 | 222.7 | 166.9 | 20 |
| Chlorthal-dimethyl (Dacthal) | 15.63 | 0.5 | 300.7 | 272.9 | 12 |
| Anthraquinone | 15.64 | 0.5 | 180 | 152 | 12 |
| Anthraquinone | 15.64 | 0.5 | 208 | 151.7 | 22 |
| Anthraquinone | 15.64 | 0.5 | 208 | 180 | 10 |
| Pyrene D10 | 15.8 | 0.5 | 212.2 | 204.1 | 60 |
| Pyrene D10 | 15.8 | 0.5 | 212.2 | 208.1 | 34 |
| Isopropalin | 16.31 | 0.5 | 280.1 | 238.2 | 8 |
| Isopropalin | 16.31 | 0.5 | 280.1 | 117.8 | 26 |
| Isopropalin | 16.31 | 0.5 | 280.1 | 180.2 | 10 |
| Isodrin | 16.49 | 0.5 | 192.9 | 123 | 28 |
| Isodrin | 16.49 | 0.5 | 146.8 | 111.1 | 10 |
| Isodrin | 16.49 | 0.5 | 192.9 | 157.2 | 20 |

**Table A3 (Part 4). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS**

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Pendimethalin | 16.5 | 0.5 | 252.1 | 161 | 14 |
| Pendimethalin | 16.5 | 0.5 | 252.1 | 162 | 8 |
| Pendimethalin | 16.5 | 0.5 | 252.1 | 191.3 | 8 |
| Heptachlor - Epoxide B | 16.78 | 0.5 | 262.9 | 192.9 | 16 |
| Heptachlor - Epoxide B | 16.78 | 0.5 | 352.8 | 252.9 | 15 |
| Heptachlor - Epoxide B | 16.78 | 0.5 | 352.8 | 262.9 | 15 |
| Fluoranthene | 17.04 | 0.5 | 202 | 200 | 32 |
| Fluoranthene | 17.04 | 0.5 | 202 | 201 | 32 |
| Fluoranthene | 17.04 | 0.5 | 202 | 152.1 | 30 |
| Chlorbenside | 17.48 | 0.5 | 125 | 89 | 16 |
| Chlorbenside | 17.48 | 0.5 | 125 | 62.8 | 28 |
| Chlorbenside | 17.48 | 0.5 | 125 | 99 | 16 |
| Chlordane gamma-*trans* | 17.53 | 0.5 | 271.7 | 236.8 | 12 |
| Chlordane gamma-*trans* | 17.53 | 0.5 | 372.7 | 263.7 | 20 |
| Chlordane gamma-*trans* | 17.53 | 0.5 | 374.7 | 265.9 | 22 |
| DDE o, p | 17.63 | 0.5 | 248.1 | 176 | 30 |
| DDE o, p | 17.63 | 0.5 | 317.8 | 248 | 18 |
| DDE o, p | 17.63 | 0.5 | 246 | 176.1 | 28 |
| Pyrene | 17.87 | 0.5 | 202 | 200 | 32 |
| Pyrene | 17.87 | 0.5 | 202 | 201 | 20 |
| Pyrene | 17.87 | 0.5 | 203 | 201 | 32 |
| Endosulfan peak 1 | 17.95 | 0.5 | 240.6 | 205.9 | 14 |
| Endosulfan peak 1 | 17.95 | 0.5 | 194.7 | 125 | 22 |
| Endosulfan peak 1 | 17.95 | 0.5 | 194.7 | 159.4 | 8 |
| Endosulfan peak 1 | 17.95 | 0.5 | 221.9 | 148 | 18 |
| Chlordane alpha-*cis* | 17.97 | 0.5 | 374.7 | 265.8 | 20 |
| Chlordane alpha-*cis* | 17.97 | 0.5 | 372.8 | 265.8 | 20 |
| Chlordane alpha-*cis* | 17.97 | 0.5 | 376.6 | 268 | 20 |
| Nonachlor-*trans* | 18.08 | 0.5 | 408.6 | 300 | 18 |
| Nonachlor-*trans* | 18.08 | 0.5 | 236.7 | 142.9 | 24 |
| Nonachlor-*trans* | 18.08 | 0.5 | 262.8 | 192.8 | 28 |
| Chlorfenson (Ovex) | 18.27 | 0.5 | 111 | 75 | 14 |
| Chlorfenson (Ovex) | 18.27 | 0.5 | 174.9 | 75 | 28 |
| Chlorfenson (Ovex) | 18.27 | 0.5 | 175 | 111 | 10 |
| DDE p, p | 18.68 | 0.5 | 317.8 | 246 | 20 |
| DDE p, p | 18.68 | 0.5 | 316 | 246 | 14 |
| DDE p, p | 18.68 | 0.5 | 246 | 176.1 | 28 |
| Dieldrin | 18.82 | 0.5 | 262.8 | 227.8 | 16 |
| Dieldrin | 18.82 | 0.5 | 276.9 | 240.9 | 12 |
| Dieldrin | 18.82 | 0.5 | 278.9 | 242.9 | 12 |
| DDD, o, p | 18.89 | 0.5 | 235 | 165.1 | 20 |
| DDD, o, p | 18.89 | 0.5 | 235 | 199 | 14 |
| DDD, o, p | 18.89 | 0.5 | 236.8 | 165 | 20 |
| Oxyfluorfen | 18.9 | 0.5 | 252 | 146 | 30 |
| Oxyfluorfen | 18.9 | 0.5 | 252 | 169.8 | 28 |
| Oxyfluorfen | 18.9 | 0.5 | 252 | 224 | 10 |

Table A3 (Part 5). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Nitrofen | 19.44 | 0.5 | 202 | 139 | 24 |
| Nitrofen | 19.44 | 0.5 | 283 | 202 | 10 |
| Nitrofen | 19.44 | 0.5 | 283 | 253 | 10 |
| Perthane (Ethylan) | 19.53 | 0.5 | 223.1 | 167 | 12 |
| Perthane (Ethylan) | 19.53 | 0.5 | 223.1 | 179 | 20 |
| Perthane (Ethylan) | 19.53 | 0.5 | 223.1 | 193 | 28 |
| Fluazifop-p-butyl | 19.54 | 0.5 | 282 | 91.1 | 18 |
| Fluazifop-p-butyl | 19.54 | 0.5 | 282 | 238.1 | 16 |
| Fluazifop-p-butyl | 19.54 | 0.5 | 383.1 | 282.1 | 14 |
| Chlorobenzilate | 19.77 | 0.5 | 139 | 111 | 12 |
| Chlorobenzilate | 19.77 | 0.5 | 111 | 75.1 | 14 |
| Chlorobenzilate | 19.77 | 0.5 | 139 | 74.9 | 26 |
| Endosulfan peak 2 | 19.83 | 0.5 | 158.9 | 123 | 12 |
| Endosulfan peak 2 | 19.83 | 0.5 | 194.7 | 159 | 8 |
| Endosulfan peak 2 | 19.83 | 0.5 | 240.6 | 205.8 | 12 |
| DDT (o, p) D8 | 20.04 | 0.5 | 243.1 | 173.1 | 22 |
| DDT (o, p) D8 | 20.04 | 0.5 | 245 | 173.1 | 22 |
| Nonachlor-*cis* | 20.04 | 0.5 | 236.8 | 142.9 | 24 |
| Nonachlor-*cis* | 20.04 | 0.5 | 262.8 | 192.9 | 28 |
| Nonachlor-*cis* | 20.04 | 0.5 | 408.7 | 300 | 18 |
| DDD, p, p | 20.05 | 0.5 | 235 | 165.1 | 20 |
| DDD, p, p | 20.05 | 0.5 | 235 | 199 | 14 |
| DDD, p, p | 20.05 | 0.5 | 236.8 | 165 | 20 |
| DDT -op | 20.14 | 0.5 | 235 | 165.1 | 20 |
| DDT -op | 20.14 | 0.5 | 235 | 199.1 | 10 |
| DDT -op | 20.14 | 0.5 | 237 | 165.1 | 22 |
| Endrin | 20.32 | 0.5 | 280.8 | 245.3 | 8 |
| Endrin | 20.32 | 0.5 | 249.8 | 214.9 | 24 |
| Endrin aldehyde | 20.86 | 0.5 | 173 | 138.1 | 16 |
| Endrin aldehyde | 20.86 | 0.5 | 278.9 | 242.9 | 10 |
| Endrin aldehyde | 20.86 | 0.5 | 344.9 | 281 | 8 |
| Methoxychlor olefin (p, p) | 20.96 | 0.5 | 238.1 | 223.1 | 10 |
| Methoxychlor olefin (p, p) | 20.96 | 0.5 | 238.1 | 152.1 | 34 |
| Methoxychlor olefin (p, p) | 20.96 | 0.5 | 308 | 238.2 | 12 |
| Endosulfan sulfate | 21.11 | 0.5 | 238.7 | 203.9 | 12 |
| Endosulfan sulfate | 21.11 | 0.5 | 271.7 | 234.9 | 12 |
| Endosulfan sulfate | 21.11 | 0.5 | 271.7 | 236.8 | 12 |
| DDT p,p | 21.31 | 0.5 | 235 | 199.5 | 10 |
| DDT p,p | 21.31 | 0.5 | 237.1 | 165.1 | 22 |
| DDT p,p | 21.31 | 0.5 | 235.1 | 165.1 | 22 |
| Carfentrazon-ethyl | 21.76 | 0.5 | 340.1 | 312.1 | 10 |
| Carfentrazon-ethyl | 21.76 | 0.5 | 311.9 | 150.7 | 18 |
| Triphenylphosphate | 21.97 | 0.5 | 326 | 325 | 5 |
| Triphenylphosphate | 21.97 | 0.5 | 77 | 51 | 10 |
| Endrin-ketone | 22.66 | 0.5 | 209.2 | 138.4 | 30 |
| Endrin-ketone | 22.66 | 0.5 | 316.8 | 208.9 | 28 |
| Endrin-ketone | 22.66 | 0.5 | 316.8 | 281 | 10 |

**Table A3 (Part 6). Selected reaction monitoring (SRM) transitions for data acquisition by GC-MS/MS**

| Name | RT | Window | Mass | Product mass | Collision energy |
|---|---|---|---|---|---|
| Chrysene | 22.95 | 0.5 | 228 | 226 | 28 |
| Chrysene | 22.95 | 0.5 | 229.1 | 227.1 | 30 |
| Chrysene | 22.95 | 0.5 | 225.9 | 223.9 | 32 |
| Chrysene D12 | 22.97 | 0.5 | 240.1 | 212.1 | 28 |
| Chrysene D12 | 22.97 | 0.5 | 236 | 232 | 28 |
| Bifenthrin | 23.03 | 0.5 | 181 | 165.9 | 10 |
| Bifenthrin | 23.03 | 0.5 | 165.1 | 163.6 | 24 |
| Bifenthrin | 23.03 | 0.5 | 181 | 179 | 12 |
| Benz[*a*]anthracene | 23.09 | 0.5 | 228 | 226 | 28 |
| Benz[*a*]anthracene | 23.09 | 0.5 | 225.9 | 223.9 | 32 |
| Benz[*a*]anthracene | 23.09 | 0.5 | 229.1 | 227.1 | 32 |
| Tetradifon | 23.87 | 0.5 | 159 | 131 | 10 |
| Tetradifon | 23.87 | 0.5 | 159 | 74.8 | 32 |
| Tetradifon | 23.87 | 0.5 | 159 | 111 | 20 |
| Phenothrin peak 1/2 | 23.95 | 0.5 | 183.1 | 168 | 12 |
| Phenothrin peak 1/2 | 23.95 | 0.5 | 183.1 | 153 | 12 |
| Phenothrin peak 1/2 | 23.95 | 0.5 | 123.1 | 81.1 | 8 |
| Mirex | 24.79 | 0.5 | 272 | 236.8 | 14 |
| Mirex | 24.79 | 0.5 | 236.8 | 142.9 | 26 |
| Mirex | 24.79 | 0.5 | 273.8 | 238.8 | 14 |
| Permethrin - *cis/ trans* | 26.42 | 0.5 | 183 | 153 | 14 |
| Permethrin - *cis/ trans* | 26.42 | 0.5 | 183 | 165.1 | 10 |
| Permethrin - *cis/ trans* | 26.42 | 0.5 | 163 | 91.1 | 12 |
| Benzo[*b*]fluoranthene | 27.36 | 0.5 | 250 | 248 | 32 |
| Benzo[*b*]fluoranthene | 27.36 | 0.5 | 252 | 250 | 32 |
| Benzo[*b*]fluoranthene | 27.36 | 0.5 | 252 | 226.1 | 28 |
| Benzo[*k*]fluoranthene | 27.47 | 0.5 | 250 | 248 | 32 |
| Benzo[*k*]fluoranthene | 27.47 | 0.5 | 252 | 250 | 32 |
| Benzo[*k*]fluoranthene | 27.47 | 0.5 | 252 | 226.1 | 28 |
| Cypermethrin peak 1 | 28 | 1 | 163 | 127.1 | 6 |
| Cypermethrin peak 1 | 28 | 1 | 163 | 91.1 | 12 |
| Cypermethrin peak 1 | 28 | 1 | 180.9 | 152.1 | 20 |
| Benzo[*a*]pyrene | 28.55 | 0.5 | 252.1 | 250 | 34 |
| Benzo[*a*]pyrene | 28.55 | 0.5 | 250 | 248 | 32 |
| Benzo[*a*]pyrene | 28.55 | 0.5 | 252 | 226.1 | 28 |
| Perylene D12 | 28.78 | 0.5 | 264 | 260.1 | 36 |
| Perylene D12 | 28.78 | 0.5 | 260.1 | 256.1 | 34 |
| Indeno[1,2,3-*cd*]pyrene | 32.49 | 0.5 | 274 | 272 | 32 |
| Indeno[1,2,3-*cd*]pyrene | 32.49 | 0.5 | 276 | 274 | 35 |
| Indeno[1,2,3-*cd*]pyrene | 32.49 | 0.5 | 138 | 124.9 | 15 |
| Dibenzo[*a,h*]anthracene | 32.64 | 0.5 | 278 | 276 | 30 |
| Dibenzo[*a,h*]anthracene | 32.64 | 0.5 | 276 | 274 | 38 |
| Dibenzo[*a,h*]anthracene | 32.64 | 0.5 | 276 | 275.1 | 26 |
| Benzo[*ghi*]perylene | 33.28 | 0.5 | 276 | 274 | 38 |
| Benzo[*ghi*]perylene | 33.28 | 0.5 | 276 | 275.1 | 23 |
| Benzo[*ghi*]perylene | 33.28 | 0.5 | 137.9 | 136.8 | 16 |

Table A4. Average, standard deviation, limit of detection LOD and LOQ from replicate analysis of 2 ng/L calibration standard

| Peak name | Average (ng/L) | Std. deviation (ng/L) | LOD (ng/L) | LOQ (ng/L) |
|---|---|---|---|---|
| Naphthalene | 2.72 | 0.97 | 2.92 | 9.75 |
| 2-methyl Napthalene | 2.72 | 0.81 | 2.42 | 8.05 |
| 1-methyl Napthalene | 2.4 | 0.43 | 1.29 | 4.31 |
| Dichlobenil | 1.83 | 0.08 | 0.23 | 0.77 |
| 3,4, Dichloroaniline | 2.03 | 0.08 | 0.25 | 0.82 |
| Acenaphthylene | 2.01 | 0.05 | 0.28 | 0.54 |
| Acenaphthene | 2.05 | 0.09 | 0.16 | 0.92 |
| Pentachlorobenzene | 1.97 | 0.07 | 0.21 | 0.71 |
| Fluorene | 1.88 | 0.14 | 0.43 | 1.42 |
| Diphenylamine | 2.09 | 0.14 | 0.41 | 1.37 |
| 2,3,5,6-Tetrachloroaniline | 1.95 | 0.06 | 0.17 | 0.58 |
| Ethalfluralin | 2.33 | 0.15 | 0.45 | 1.49 |
| Trifluralin | 2.21 | 0.08 | 0.24 | 0.79 |
| Benfluralin | 2.26 | 0.10 | 0.3 | 0.99 |
| HCH - alpha | 1.96 | 0.04 | 0.11 | 0.38 |
| Hexachlorobenzene | 1.92 | 0.10 | 0.3 | 0.99 |
| Pentachloroanisole | 1.92 | 0.05 | 0.14 | 0.47 |
| HCH - beta | 1.93 | 0.09 | 0.27 | 0.9 |
| HCH - gamma (lindane) | 1.96 | 0.10 | 0.29 | 0.97 |
| Pentachloronitrobenzene | 2.25 | 0.08 | 0.23 | 0.77 |
| Phenanthrene | 1.68 | 1.18 | 3.54 | 11.8 |
| Chlorothalonil | 1.96 | 0.1 | 0.29 | 0.98 |
| Anthracene | 2.06 | 0.08 | 0.24 | 0.82 |
| HCH - delta | 2.04 | 0.09 | 0.26 | 0.87 |
| Endosulfan ether | 1.7 | 0.12 | 0.37 | 1.22 |
| Transfluthrin | 176 | 0.09 | 0.28 | 0.95 |
| Heptachlor | 1.41 | 0.17 | 0.51 | 1.71 |
| Prodiamine | 1.89 | 0.18 | 0.55 | 1.82 |
| Pentachlorothioanisole | 2.11 | 0.12 | 0.36 | 1.21 |
| Aldrin | 2.3 | 0.25 | 0.76 | 2.55 |
| Anthraquinone | 1.69 | 0.21 | 0.62 | 2.08 |
| Chlorthal-dimethyl (Dacthal) | 1.91 | 0.05 | 0.14 | 0.47 |
| Isopropalin | 2.07 | 0.12 | 0.37 | 1.24 |
| Isodrin | 2.24 | 0.19 | 0.58 | 1.94 |
| Pendimethalin | 2.21 | 0.14 | 0.42 | 1.40 |
| Heptachlor - Epoxide B | 1.93 | 0.16 | 0.47 | 1.57 |
| Fluoranthene | 1.92 | 0.44 | 1.31 | 4.36 |
| Chlorbenside | 2.09 | 0.08 | 0.25 | 0.84 |
| Chlordane gamma-*trans* | 1.78 | 0.1 | 0.3 | 1.02 |
| DDE o, p | 1.97 | 0.17 | 0.52 | 1.72 |
| Pyrene | 1.54 | 0.27 | 0.82 | 2.73 |
| Endosulfan peak 1 | 2.01 | 0.09 | 0.28 | 0.94 |
| Chlordane alpha-*cis* | 1.73 | 0.21 | 0.63 | 2.11 |
| Nonachlor-*trans* | 2.09 | 0.32 | 0.96 | 3.18 |
| Chlorfenson (Ovex) | 2.04 | 0.07 | 0.22 | 0.75 |
| DDE p, p | 1.97 | 0.16 | 0.47 | 1.58 |
| Dieldrin | 1.05 | 0.28 | 0.85 | 2.85 |
| DDD, o, p | 1.64 | 0.07 | 0.2 | 0.67 |
| Nitrofen | 2.61 | 0.18 | 0.54 | 1.8 |
| Perthane (Ethylan) | 1.78 | 0.21 | 0.73 | 2.45 |
| Fluazifop-p-butyl | 1.58 | 0.18 | 0.53 | 1.76 |
| Endosulfan peak 2 | 1.36 | 0.25 | 0.74 | 2.45 |
| DDD, p, p | 1.94 | 0.09 | 0.56 | 1.87 |
| Nonachlor-*cis* | 2.19 | 0.19 | 0.27 | 0.9 |
| DDT -op | 2.03 | 0.1 | 0.29 | 0.96 |
| Endrin | 1.62 | 0.24 | 0.71 | 2.35 |
| Methoxychlor olefin (p, p) | 1.69 | 0.04 | 0.13 | 0.43 |
| Endosulfan sulfate | 1.56 | 0.12 | 0.35 | 1.16 |
| DDT p,p | 1.42 | 0.94 | 2.81 | 9.35 |
| Endrin-ketone | 1.72 | 0.08 | 0.24 | 0.8 |
| Chrysene | 2.04 | 0.06 | 0.18 | 0.6 |
| Bifenthrin | 2.17 | 0.16 | 0.49 | 1.62 |
| Benz[*a*]anthracene | 2.17 | 0.13 | 0.38 | 1.26 |
| Tetradifon | 2.00 | 0.27 | 0.82 | 2.73 |
| Phenothrin peak 2 | 1.87 | 0.4 | 1.21 | 4.05 |
| Mirex | 1.99 | 0.35 | 1.05 | 3.49 |
| Permethrin - *cis* | 2.2 | 0.08 | 0.24 | 0.8 |
| Permethrin - *trans* | 2.39 | 0.21 | 0.64 | 2.12 |
| Benzo[*b*]fluoranthene | 2.27 | 0.08 | 0.25 | 0.82 |
| Benzo[*k*]fluoranthene | 2.24 | 0.13 | 0.4 | 1.34 |
| Cypermethrin peak 1 | 2.41 | 0.19 | 0.58 | 1.95 |
| Cypermethrin peak 2 | 2.00 | 0.15 | 0.44 | 1.46 |
| Cypermethrin peak 3 | 2.03 | 0.21 | 0.63 | 2.09 |
| Cypermethrin peak 4 | 2.01 | 0.08 | 0.25 | 0.84 |
| Benzo[a]pyrene | 2.24 | 0.29 | 0.87 | 2.9 |
| Indeno[1,2,3-*cd*]pyrene | 2.17 | 0.19 | 0.56 | 1.9 |
| Dibenzo[*a,h*]anthracene | 2.25 | 0.24 | 0.73 | 2.42 |
| Benzo[*ghi*]perylene | 2.16 | 0.16 | 0.49 | 1.64 |

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