Improved laboratory productivity with a single GC-MS/MS configuration for multipurpose environmental analysis

Authors

Delphine Thomas, Bénédicte Gauriat

Thermo Fisher Scientific Customer Solution Center, Les Ulis, France

Keywords

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Goal

This application note will highlight a single instrument configuration, based on triple quadrupole GC-MS, to perform the analysis of various compound classes commonly monitored in the environment. This will allow laboratories to standardize on a single hardware configuration and hence greatly facilitate laboratory capacity, instrument- and consumables management, as well as streamlining staff training.

Introduction

Analytical testing laboratories play a pivotal role in monitoring common contaminants in different matrices. While data quality and compliance with established regulated methods is key in ensuring a laboratory's reputation, productivity and fast sample turnover times are equally important to ensure profitable operation.

In the field of environmental monitoring, a large variety of compound classes may be required for analysis, including both common and emerging contaminants. For volatile and semi-volatile substances, gas chromatography is the method of choice for separating pesticides, polyaromatic hydrocarbons (PAHs), flame retardants such as polybrominated diphenyl ethers (PBDEs), and others. In many cases, due to previously existing methodologies, samples need to undergo several analyses on different instrument configurations, with either specific consumables, including the analytical column or a dedicated detector. This leads to a variety of protocols and potential instrument setups required in a laboratory, some of which must be run in a dual-column configuration or a confirmation on a separate instrument using a second injection is required.

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While mass spectrometric detection provides a much higher selectivity than analog detectors, only triple quadrupole systems provide the selectivity needed to effectively leverage selected rection monitoring (SRM) as a tool for method standardization and consolidation. The power of triple quadrupole mass spectrometry can be easily used to modernize existing workflows. Laboratories can reduce their need for instrument-specific consumables and components on-hand to reduce costs and complexity with a single instrument configuration. This application demonstrates the use of a single hardware configuration for the analysis of different environmental contaminants.

Experimental

For all measurements, a Thermo Scientific™ TRACE™ 1610 GC coupled to Thermo Scientific™ TSQ™ 9610 GC-MS/MS was used. The system was equipped with a Thermo Scientific™ iConnect™ Thermospray SSL Injector Module (TSI).

The analytical column used for all substance classes was a Thermo Scientific™ TraceGOLD™ TG-Contaminants GC column, which allows for fast analysis of multi-class contaminants including pesticides, polychlorinated biphenyls (PCBs), PAHs, and PBDEs. These highly inert capillary columns combine thermal stability with a unique selectivity to ensure excellent chromatographic peak shapes and sensitivity and allow chromatography of semi-volatile compounds together with late-eluting compounds. Table 1 gives a high-level summary of the parameters for each of the three methods showcased.

Single GC-MS/MS configuration

- Thermo Scientific™ TriPlus™ RSH SMART autosampler (P/N 1R77010-2003)
- TRACE GC 1610 (P/N MI-148000-0007)
- Thermospray injector TSI (P/N 19070016)
- TSQ 9610 AEI source (P/N TSQ9610-NV-AEI)
- TraceGOLD TG-Contaminants GC column 15 m × 0.25 mm × 0.1 µm (P/N 26056-0350)
- Thermo Scientific™ LinerGOLD™ splitless precision liner, quartz wool (P/N 453T2999-UI)

Figure 1 gives detailed information on the configuration used for the analysis.

Table 1. Instrument parameters

Parameter	PBDE	Pesticides			Micropollutants
Injection mode	Splitless	Split with surge			Split
Injection volume (µL)	2 µL	3 µL			2 µL
GC run time (min)	16 minutes	20 minutes			20 minutes
Number of compounds monitored	9	350			220
Calibration range in solvents (µg/L)	1 to 500	2 to 250			2 to 250
Compound classes covered	• Flame retardants	•Carbamates •Triazines •Azoles •Ureas	•Organochlorides •Organophosphorous •Organonitrogens •Pyrethroids	•Morpholines •Anilides •Uracils •Amides •Strobilurins	•PCBs •Phenolic derivatives •PAHs •Aniline derivatives •Benzene derivatives
Acquisition mode	SRM				

For further information, contact your local commercial representative

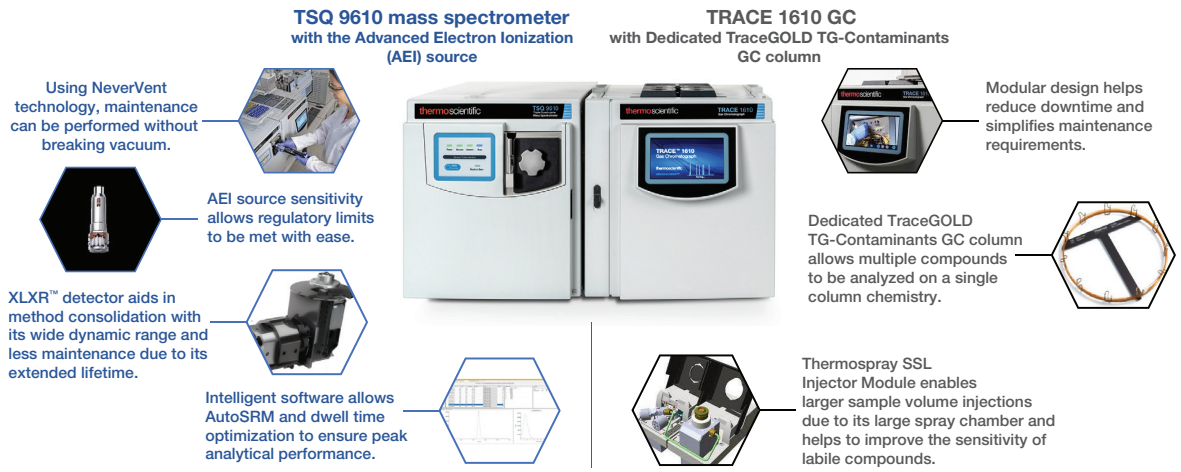

Figure 1. Configuration utilized for analysis the TRACE 1610 GC with the TSQ 9610 NV-AEI GC-MS/MS

Results and discussion

Analysis of polybrominated diphenylethers (PBDE)

PBDEs are used as additive flame retardants in different materials and can leach into the environment where they persist and bioaccumulate.[1] PBDEs are a class of brominated hydrocarbons with a basic structure containing two phenyl rings linked by an oxygen atom. Within the European Standard 16694:2025, applicable for water analysis, the determination of six selected PBDEs is required, which include congeners BDE-28, -47, -99, -100, -153, and -154.

The proposed setup has been tested to comply with the requirements, using the conditions summarized in Table 1.

In addition to the required congeners, BDEs 183, 207, and 209 also have been monitored; they can be separated and quantified at required levels, as is demonstrated by the selected reaction monitoring plot shown in Figure 2. Figure 3 shows a more detailed SRM plot for BDE-28, BDE-99, and BDE-183. These plots show that four SRM transitions are clearly visible at this concentration, which aids in confirming the presence of the compounds in an environmental sample.

To demonstrate the performance, the chromatograms shown in Figure 3 present three examples of PBDE compounds at 1 µg/L in solvent using SRM analysis.

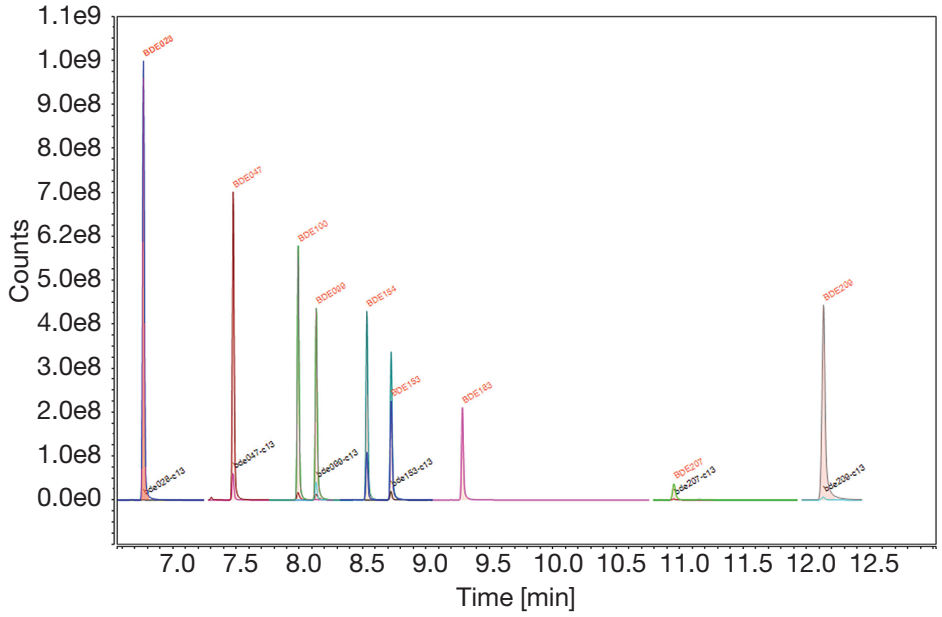

Figure 2. SRM plot for the separation of PBDEs at a concentration of 1 ppm, in line with the requirements of European Standard 16694:2015

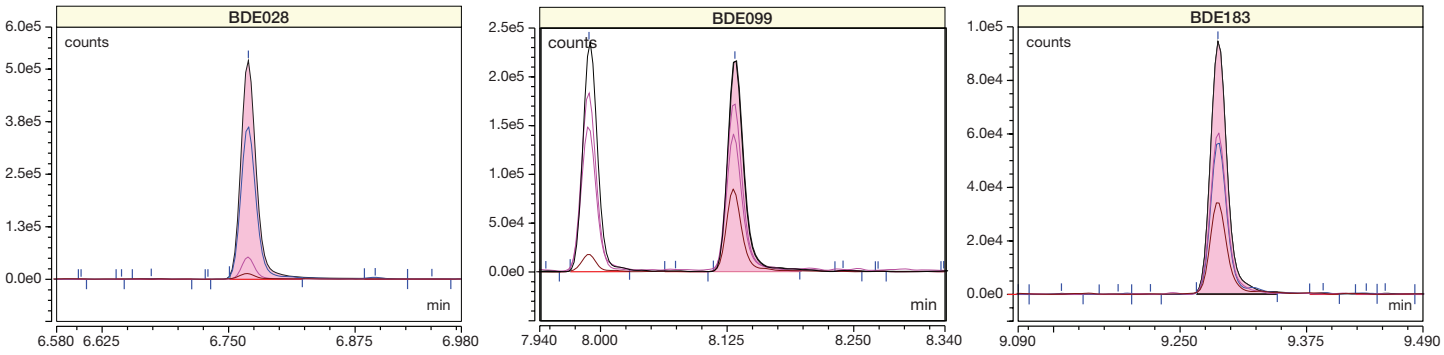

Figure 3. Overlaid SRM traces at 1 µg/L (quantifier and qualifier)

Analysis of pesticides

Even though pesticides are commonly analyzed in food samples, they also need to be determined in water samples to ensure that they do not contaminate waterways and in turn have a negative effect on the ecosystem. One example of a regulation to monitor pesticides in water is the European Groundwater Directive (2006/118/EC).

Approximately 1,000 active substances are currently used in pesticide formulations. In addition, metabolites, degradation products, and ‘‘old’’ (persistent) pesticides must be considered by pesticide residue analysts. Pesticides have different chemical and physical properties but can be grouped into multiple sub-classes, i.e., organophosphorus compounds, pyrethroids, organochlorides, carbamates, and azoles.

Using the proposed methodology, described in more detail elsewhere,[2,3] up to 350 individual pesticides can be analyzed, covering a wide range of compound classes. A full overview of the entire separation is given in Figure 4.

Figure 5 shows examples of SRM chromatograms for five pesticide compounds (class of organophosphorus, pyrethroid, organochloride, carbamate, and azole) at a concentration of 3 µg/L.

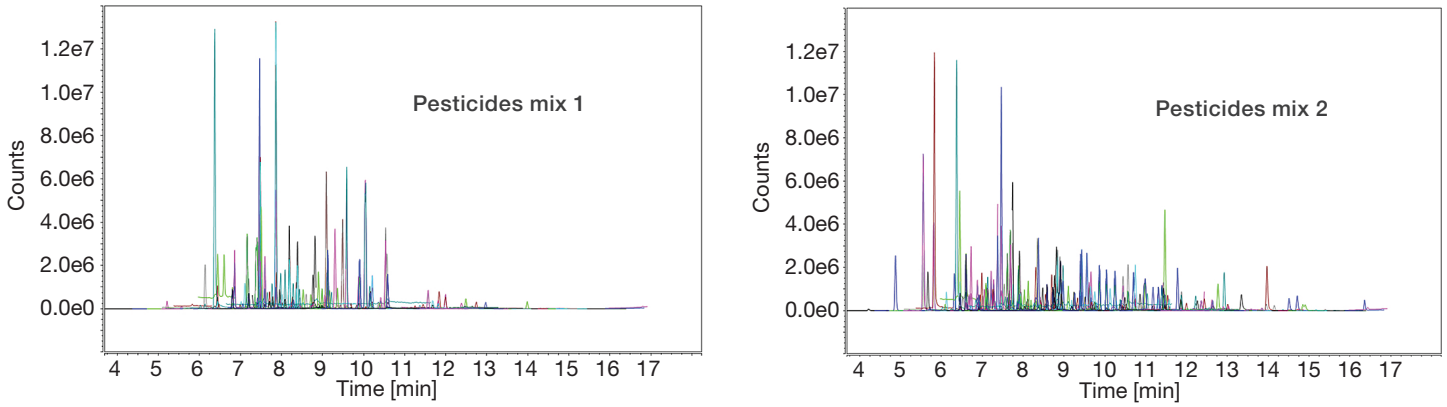

Figure 4. Two SRM plots of two mixtures of pesticides covering 350 compounds at a concentration of 10 ppb, showing good separation within 20 minutes

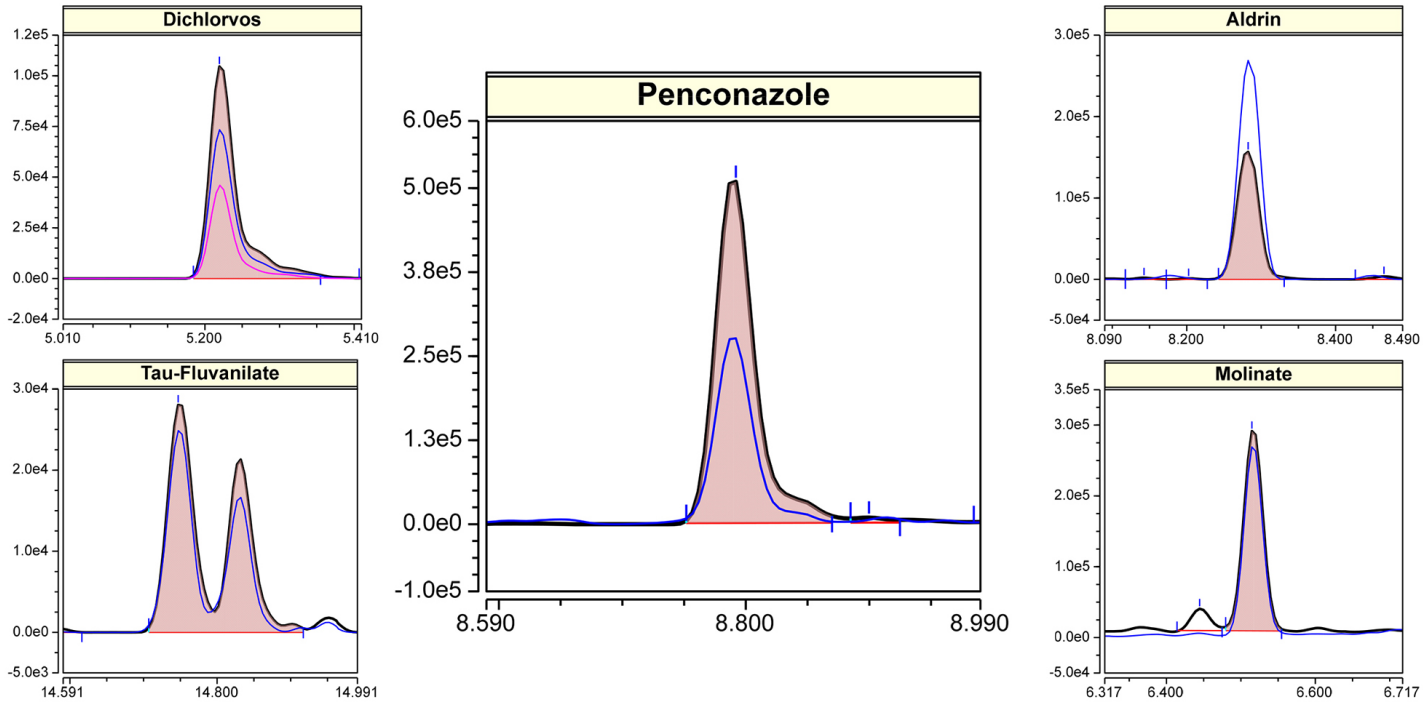

Figure 5. Selected pesticides chromatograms at 3 µg/L

Analysis of micropollutants

The term micropolluntants describes different, mostly organic, chemicals that may enter the environment from anthropogenic processes. A main source for micropollutants is wastewater from all sources, including industrial plants, agricultural processes, and private households. Even though micropollutants are present in low concentrations, long-term exposure may pose considerable risks to aquatic organisms and human health. Micropollutants can be separated into a variety of compound classes, out of which a great number are amenable to gas chromatographic analysis.

An example of an SRM chromatogram for the full method including all the classes under evaluation is given in Figure 6.

In Figure 7, chromatograms summarize five representive examples across all compound classes included in the method, namely derivatives of phenolics, benzenes, anilines, PCBs, and PAHs. Each compound was present in the mix at a concentration of 5 µg/L. 2-chlorophenol, nitrobenzene, pentachloroaniline, 1,5-dichloronaphthalene, and PCB209 were selected as representative compounds of the compound classes.

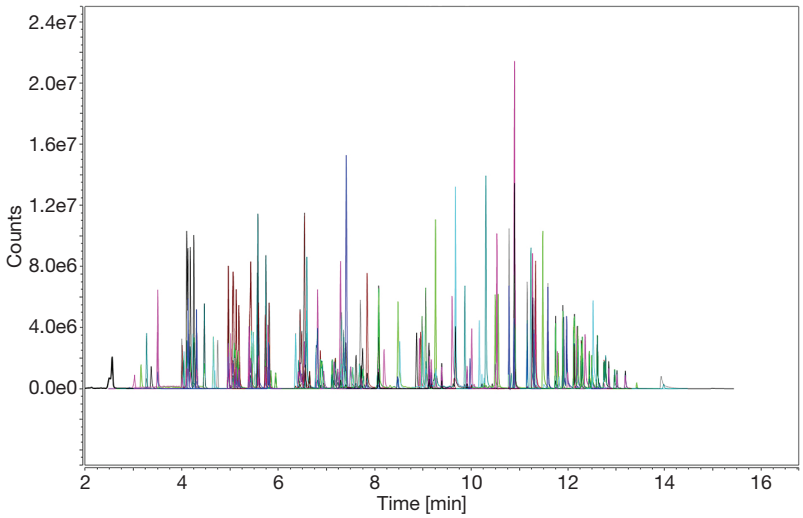

Figure 6. SRM plot of the micropollutants full method at a concentration of 50 ppb

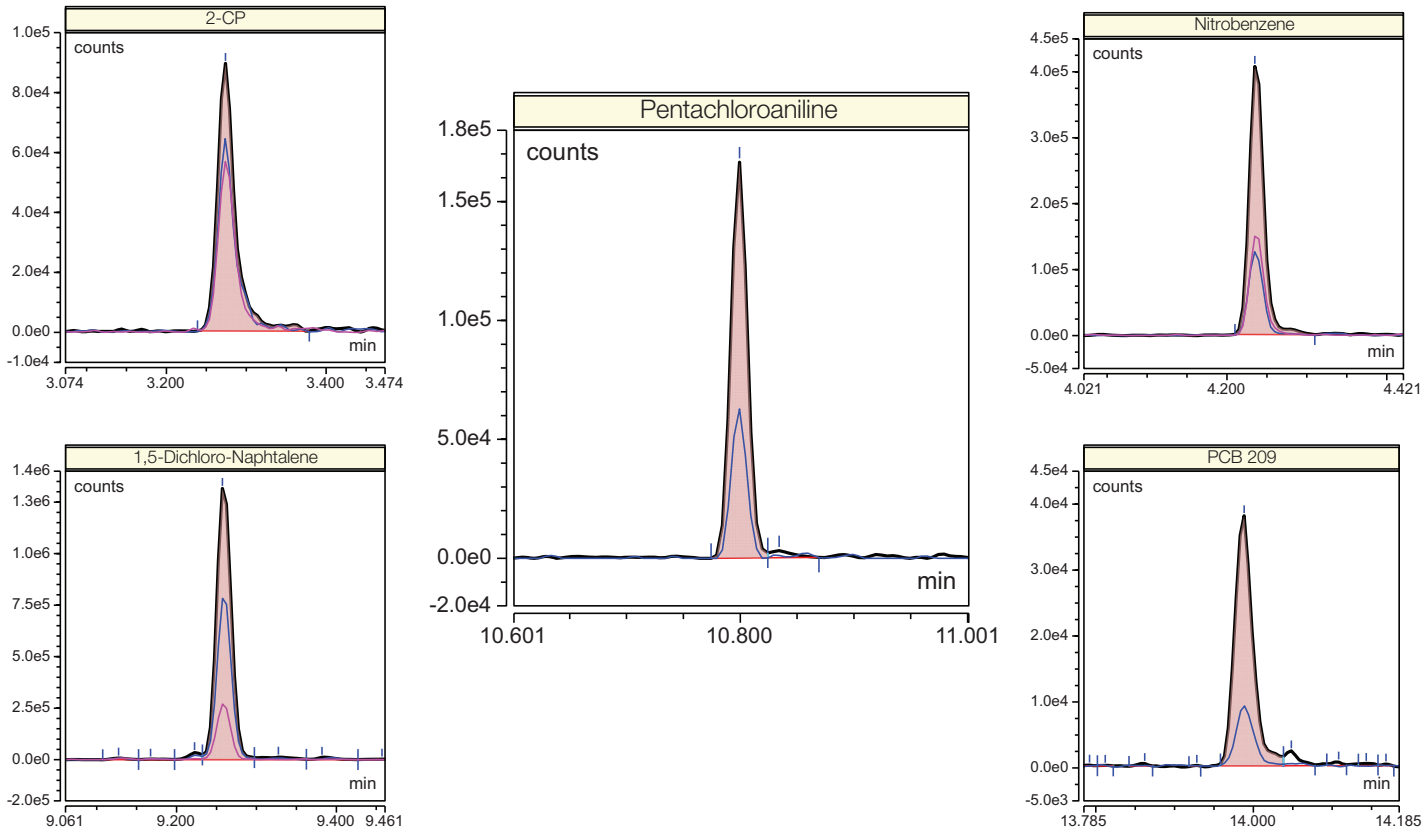

Figure 7. Overlaid SRM traces at 5 µg/L (quantifier and qualifier)

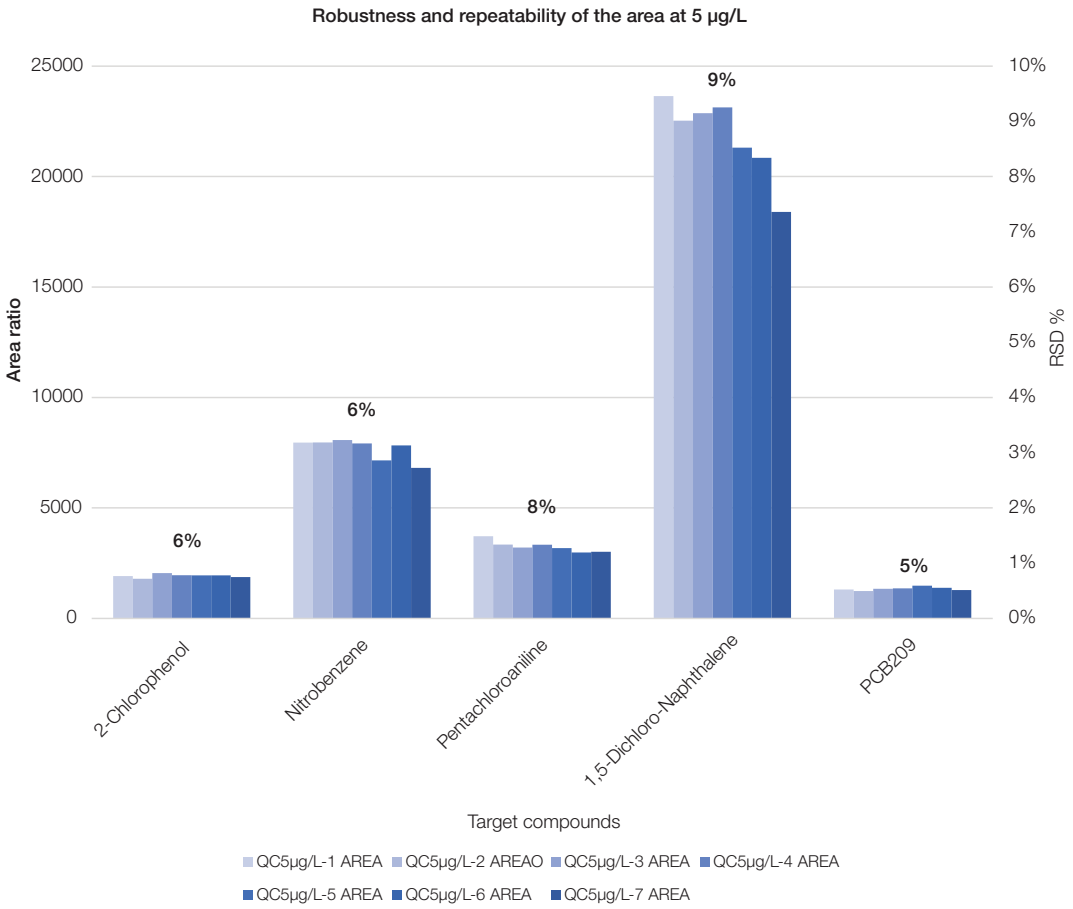

Figure 8. Peak area %RSD obtained for the QC checks at 5 µg/L (n=7), analyzed before and after the repeated injection of matrix samples (n=80)

To illustrate the robustness and repeatability of the method, the average peak area determined for all compounds covered in the method was evaluated. This was accomplished using QC check standards at 5 µg/L, injected before and after the analysis of 80 water samples. No maintenance or tuning was performed on either the inlet system or the mass spectrometer. The results are displayed in Figure 8.

Conclusion

The utilization of a single configuration GC-MS/MS for multiple environmental methods has been demonstrated in this application note. As well as being able to meet the regulatory requirements for different compound classes, there are advantages to using a single configuration for multiple analysis:

- Reduction in operation cost, including reduced training needs and centralization of consumables
- Ability to react and be ready to run the required method without lengthy set up or changing instrument analytical column and hardware
- Increase in instrument capacity as all systems can run all methods

The Thermo Scientific GC-MS/MS system also increases productivity:

- The TRACE 1610 GC has a unique module design allowing injectors and detectors to be exchanged by the user and maintenance to be performed rapidly offline. The TSI injector allows a wider range of compound classes with different volatilities to be covered in a single injection. The easy-to-use touch screen provides real-time monitoring of the system and video tutorials for quick adoption.
- The TSQ 9610 GC-MS/MS is equipped with Thermo Scientific™ NeverVent™ technology, which allows the GC column to be exchanged, the ionization source to be removed, and filaments to be removed without the need for breaking vacuum. This allows routine maintenance to be performed in minutes and increases system uptime drastically.

In summary, this single GC-MS/MS configuration can greatly simplify the workflows of environmental laboratories and increase efficiency and productivity, reduce costs, and maximize revenue.

References

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