Environmental

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

Amit Gujar[1], Delphine Thomas[2] and Bénédicte Gauriat[2]
[1]Thermo Fisher Scientific, USA, [2]Thermo Fisher Scientific, CSC, France

Abstract

Purpose: Very often the analysis of various compound classes commonly monitored in the environment leads analytical testing laboratories to set up and validate multiple procedures using different instrument configurations. The adoption of a single instrument configuration would therefore greatly improve laboratory capacity, instrument- and consumables management, as well as streamlining staff training.
Methods: The multi-residual analysis of PBDEs, pesticides and micropollutants was consolidated on a single analytical platform consisting of a triple quadrupole GC-MS/MS equipped with a Thermospray SSL Injector.
Results: The utilization of a single instrument configuration for the analysis of multiple compound classes in environmental samples allowed to meet the regulatory requirements while reducing the operational costs, including reduced training needs and centralization of consumables, as well as increasing the productivity.

Introduction

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 coupled to mass spectrometry is the method of choice for separating pesticides, polyaromatic hydrocarbons (PAHs), flame retardants such as polybrominated diphenyl ethers (PBDEs), and others.
In many cases, a variety of protocols and potential instrument setups are required for the analysis. Triple quadrupole systems provide the selectivity needed to effectively leverage the selected rection monitoring (SRM) acquisition 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.

Materials and methods

Test Method

A Thermo Scientific™ TRACE™ 1610 GC equipped with a Thermo Scientific™ iConnect™ Thermospray SSL Injector Module (TSI) and coupled to Thermo Scientific™ TSQ™ 9610 GC-MS/MS (Figure 1) was used for the analysis of multiple classes of contaminants such as pesticides, PBDEs, PAHs and micropollutants (Table 1).

Data Analysis

Data was acquired, processed, and reported using the Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software, version 7.3.

Figure 1. Instrument configuration

Table 1. Instrument parameters

Parameter	PBDE	Pesticides	Micropollutants
Injection mode	Splitless	Split with surge	Split
Injection volume (µL)	2	3	2
GC run time (min)	16	20	20
Monitored compounds (n)	9	350	220
Calibration range in solvent (µg/L)	1-500	2-250	2-250
Compound classes	•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		

Results

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. 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. In addition to the required congeners, BDEs 183, 207, and 209 were also monitored, expanding the list of the target compounds. All the compounds could be separated and quantified at required levels (Figure 2). The typical PBDE quantifier and qualifier ion transitions were clearly visible at a concentration of 1 µg/L therefore adding more confidence in confirming the presence of the compounds in the environmental samples. Some examples for BDE-28, BDE-99, and BDE-183 are reported in Figure 3.

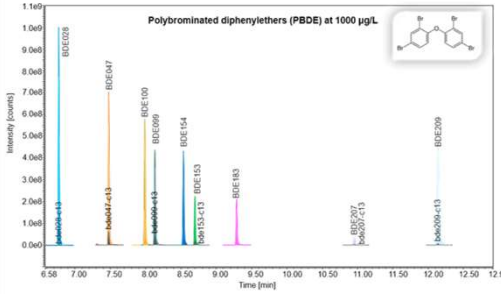

Figure 2. SRM chromatogram showing the chromatography of a PBDE mix at a concentration of 1000 µg/L, meeting the requirements of European Standard 16694:2015

Download full application note here

Analysis of pesticides

Even though pesticides are commonly analyzed in food samples, they also need to be determined in water samples to ensure they do not contaminate waterways and in turn have a negative effect on the ecosystem. Approximately 1,000 active substances are currently used in pesticide formulations. In addition, metabolites, degradation products, and persistent pesticides must be considered in multiresidue analysis. Pesticides are heterogenous compounds with different chemical and physical properties and therefore classified into multiple sub-classes, i.e., organophosphorus compounds, pyrethroids, organochlorides, carbamates, and azoles.

The use of the proposed configuration working in SRM acquisition mode allowed to detected and confirm up to 350 individual pesticides belonging to a wide range of compound classes. Some examples of quantifier and qualifier ions at a concentration of 3 µg/L for the most representative pesticides among organophosphorus, pyrethroid, organochloride, carbamate, and azole classes are reported in Figure 4.

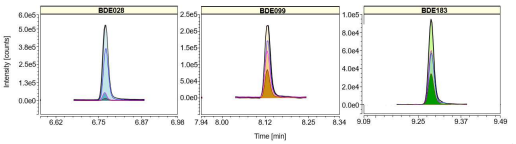

Figure 3. Examples of overlaid quantifier (outlined in black) and qualifier ions at 1 µg/L

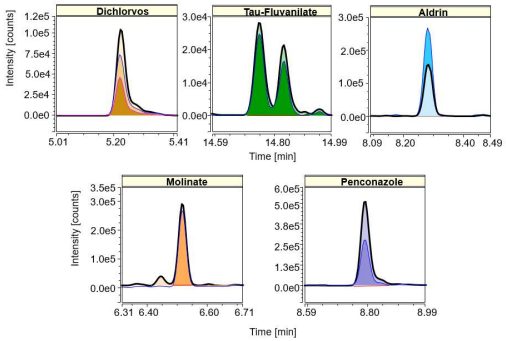

Figure 4. Examples of overlaid quantifier (outlined in black) and qualifier ions for some representative pesticides at 3 µg/L

Analysis of micropollutants

The term micropollutants describes different chemicals that may enter the environment from anthropogenic processes. Wastewater from all sources including industrial, plants, agricultural processes and private households can contain traces of micropollutants . Even though these are present at low concentrations, long-term exposure may pose considerable risks to aquatic organisms and human health. Micropollutants can be classified in a variety of compound classes, out of which a great number are amenable to gas chromatographic analysis due to their volatility. Five representative compounds of the investigated compound classes (phenolics, benzenes, anilines, PCBs, and PAHs) are reported in Figure 5.

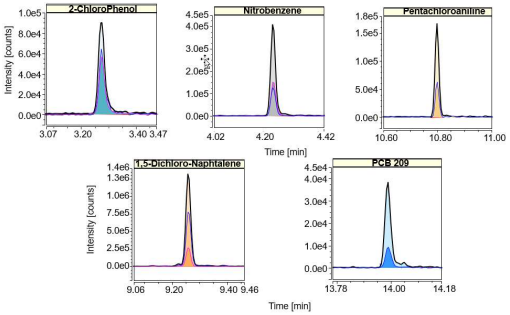

Figure 5. Examples of overlaid quantifier (outlined in black) and qualifier ions at 5 µg/L

Conclusions

The utilization of a single configuration GC-MS/MS for multiple environmental methods allowed to meet the regulatory requirements for different compound classes offering the advantages of:

- Reduction in operational costs, 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
- Increased instrument capacity and laboratory productivity.

References

1. Hites, R.A. Polybrominated diphenyl ethers in the environment and in people: a meta-analysis of concentrations. Environ. Sci. Technology 2004, 38, 945.
2. Thermo Fisher Scientific Application Brief AB00019: Improving the routine testing of difficult-to-analyze pesticide residues by using the Thermo Scientific TraceGOLD TG-Contaminants column with GC-MS/MS technology. https://assets.thermofisher.com/TFS-Assets/CMD/Application-Notes/ab-000019-gcms-div-ctl-tg-contaminants-ab000019-en.pdf
3. Thermo Fisher Scientific Application Note AN00780: A robust and sensitive method for the determination of pesticides in surface and ground water by triple quadrupole GC-MS. https://assets.thermofisher.com/TFS-Assets/CMD/Application-Notes/an-000780-gc-ms-tsq-9610-pesticides-groundwater-an000780-na-en-1.pdf

Trademarks/licensing

© 2024Thermo Fisher Scientific Inc. All rights reserved. All trademarks are the property of Thermo Fisher Scientific and its subsidiaries unless otherwise specified. This information is not intended to encourage use of these products in any manner that might infringe the intellectual property rights of others.

Learn more at thermofisher.com/TSQ9610