



Thermo Scientific Water Analysis

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# Compliance and Workflows European Water Framework Directive

2013/39/EU

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# An introduction to the 2013/39/EU Directive

Many chemicals produced by human industrial activities have a negative impact on the aquatic environment, even at extremely low concentrations. Some very hydrophobic substances accumulate in biota and are therefore not detected in water alone. To measure such an effect, many environmental chemists aim to develop analytical methodologies that can identify a substance at the intended Environmental Quality Standard (EQS) level in complex environmental matrices, including biota.

For this reason, the directive 2013/39/EU introduced in August 2013 provides a strategy to monitor pollution of water and biota for European Union member states. This strategy involves the identification of priority substances that pose a significant risk to the aquatic environment. It amends Directives 2000/60/EC and 2008/105/EC regarding a common implementation policy to protect water bodies against pollution, committing all member states to actively control and monitor the water bodies for a long list of environmental contaminants.

The list of compounds to be monitored includes different classes of contaminants such as pesticides, brominated flame retardants, perfluorinated compounds, dioxins, phenols, and metals. Directive 2013/39/EU also contains the first watch list for Union-wide monitoring for a pharmaceutical compound (diclofenac) and two steroid hormones (17-beta-estradiol, 17-alpha-ethinylestradiol).

For the purpose of analyzing such a range of contaminants, different analytical methodologies are suggested. The complete range of Thermo Scientific™ systems covers every step of the workflow requirements, from sample preparation to analysis and reporting.

# List of Contaminants Monitored and Recommended Methods of Analysis

Analysis Method			
Substance	GC-MS	LC-MS	ICP-MS
<b>Priority Hazardous Substances – considered extremely harmful</b>			
Anthracene	•		
Brominated Diphenylethers	•		
Cadmium and its compounds			•
C10-13 Chloroalkanes		•	
Di-(2-ethylhexyl)phthalate (DEHP)	•		
Endosulfan	•		
Hexachlorobenzene (HCB)	•		
Hexachlorobutadiene (HCBDD)	•		
Hexachlorocyclohexane	•		
Mercury and its compounds			•
Nonylphenols	•		
Pentachlorobenzene	•		
Polyaromatic Hydrocarbons (PAHs)	•		
Tributyltin compounds	•		• *
Trifluralin	•		
Dicofol	•		
Perfluorooctane sulfonic acid and its derivatives (PFOS)		•	
Quinoxifen		•	
Dioxins and Dioxin-like compounds	•		
Hexabromocyclododecanes (HBCDD)	•	•	
Heptachlor and heptachlor epoxide	•		

\* requires Thermo Scientific™ TRACE™ 1300 GC

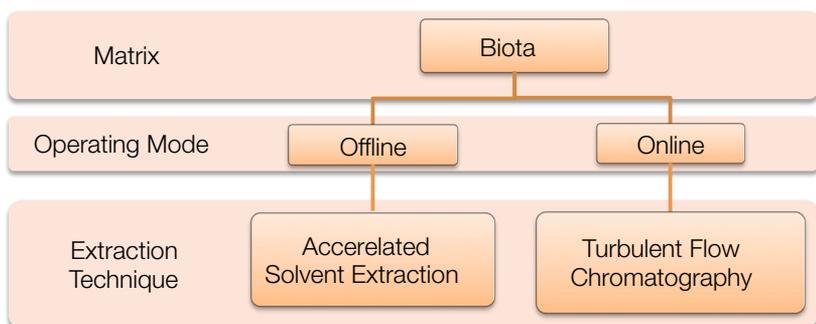
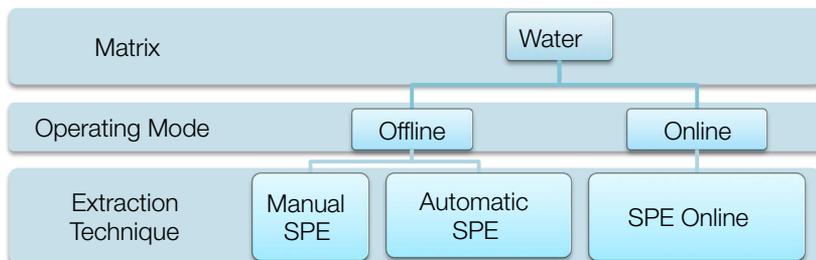
Analysis Method			
Substance	GC-MS	LC-MS	ICP-MS
<b>Priority Substances – considered harmful</b>			
Alachlor	•		
Atrazine		•	
Benzene	•		
Chlorfenvinphos		•	
Chlorpyrifos (ethyl)	•		
1,2-dichloroethane	•		
Dichloromethane	•		
Diuron		•	
Fluoranthene	•		
Isoproturon		•	
Lead and its compounds			•
Naphthalene	•		
Nickel and its compounds			•
Octylphenols	•		
Pentachlorophenol	•		
Simazine		•	
Trichlorobenzenes	•		
Trichloromethane (chloroform)	•		
Aclonifen	•		
Bifenox	•		
Cybutryne	•		
Cypermethrin	•		
Dichlorvos	•		
Terbutryn	•	•	
<b>Watch List – substances to be monitored in order to gather information on the risk those substance pose to the environment</b>			
Diclofenac		•	
17-beta-estradiol	•	•	
17-alpha-ethinylestradiol	•	•	

# Sample Preparation



Monitoring water status requires understanding the entire matrix, including not only different water sources, but also biota and sediments. Extraction techniques such as solid phase extraction (SPE), accelerated solvent extraction (ASE), and turbulent flow chromatography are techniques of choice when managing difficult environmental matrices in an efficient way.

A variety of manual and automated Thermo Scientific accessories and systems are available to simplify and resolve sample preparation requirements.



Automated and semi-automated techniques associated with the analysis of both water and biota.



Solid phase extraction cartridges

## Solid Phase Extraction (SPE)

The choice of SPE sorbent depends on the following attributes:

- Physicochemical differences between the analyte and matrix
- Analyte solubility
- Analyte polarity (LogP/LogD)
- Analyte charge state (pKa analyte/pH of solution)





### Automated SPE

The Thermo Scientific™ Dionex™ AutoTrace™ 280 Solid-Phase Extraction instrument automates cartridge or disk conditioning, sample loading, rinsing, and eluting steps for large-volume aqueous solution extractions (20 mL to 20 L).

#### Benefits:

- Reduced solvent usage and elimination of glassware
- Does not require technician involvement to control the flow of organic solvent through the SPE cartridge
- No hood required
- Provides constant flow of liquids through SPE cartridges



Dionex AutoTrace 280  
SPE Instrument

### Accelerated Solvent Extraction (ASE)

The Thermo Scientific™ Dionex™ ASE™ 350 Accelerated Solvent Extractor is a proprietary system for the extraction of solid and semi-solid samples employing commonly used solvents at elevated temperatures and pressures.

#### Benefits:

- Automatically extracts up to 24 samples, 1–100 g each, in 10–20 min per sample
- Solvent use reduced to as low as 5 mL per sample
- Can cover wide range of applications such as PAHs, PCBs, and Brominated Flame Retardants
- Handles acidic and alkaline pre-treated matrices
- Approved for EPA Method 3545A and CLP Program



Accelerated Solvent Extractor

### EQuan MAX Plus System

The Thermo Scientific™ EQuan MAX Plus™ System is an automated, high-throughput LC-MS solution for water analysis.

#### Benefits:

- Full compatibility with both LC-MS/MS and LC-HRMS
- Direct analysis of water samples (up to 20 mL)
- Extraction times reduced to minutes



EQuan MAX Plus System

### Turbulent Flow Technology

Thermo Scientific™ TurboFlow™ technology combines diffusion, chemistry, and size exclusion to perform selective online sample clean up of dirty or difficult matrices prior to HPLC or UHPLC separation and MS analysis.

#### Benefits:

- Reduces sample preparation time—direct LC-MS analysis
- Minimizes matrix effects
- Multiplexing capabilities

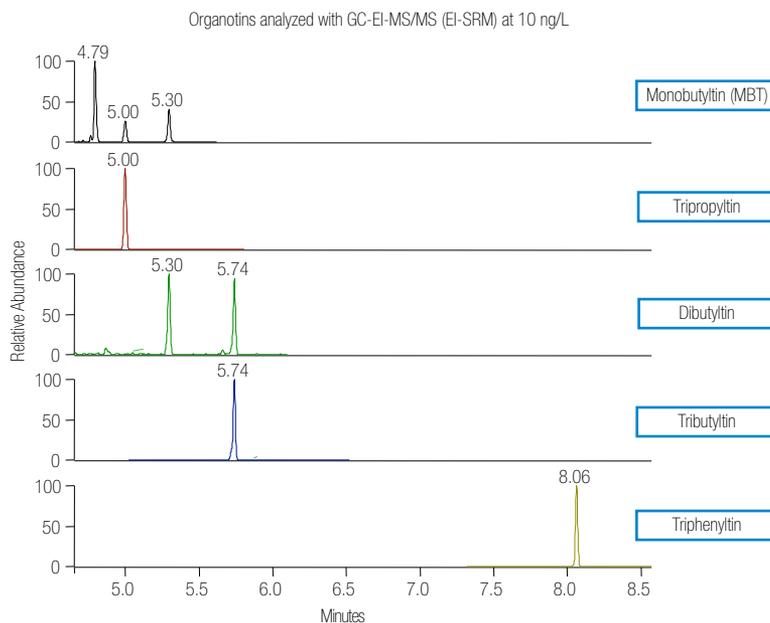


Thermo Scientific™  
Transcend™ II System with  
Multiplexing Turboflow  
Technology

# GC Amenable Contaminants: Recommended Configurations

Group	Thermo Scientific™ TriPlus™ RSH Autosampler	Thermo Scientific™ TRACE™ 1300/1310 Series GC	MS Analyzer (Acquisition Mode)
VOC	Headspace	SSL or PTV	Thermo Scientific™ ISQ™ Single Quadrupole GC-MS or Thermo Scientific™ TSQ™ series GC-MS/MS* (EI-Timed SIM)
BDE	LV option	PTV	TSQ series GC-MS/MS* (EI-SRM or NCI-SIM)
Organotin compounds	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM) Tributyltin: Thermo Scientific™ iCap Q ICP-MS
Polychlorinated Alkanes	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM)
Dioxins/Dioxin-like compounds	TriPlus 100 LS	SSL or PTV	Thermo Scientific™ DFS™ GC-HRMS
Pesticides	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM)
PAHs	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM)
Phenols	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM)
Phthalates	TriPlus 100 LS	PTV	TSQ series GC-MS/MS* (EI-SRM)

\* TSQ series GC-MS/MS includes the TSQ Duo system, which provides superior performance in both single and triple quadrupole modes and the TSQ 8000 Evo system, our highest performance GC-MS/MS instrument for high throughput laboratories.



Examples of GC-MS/MS chromatograms at 2 ng/mL.

# LC Amenable Contaminants: Recommended Configurations

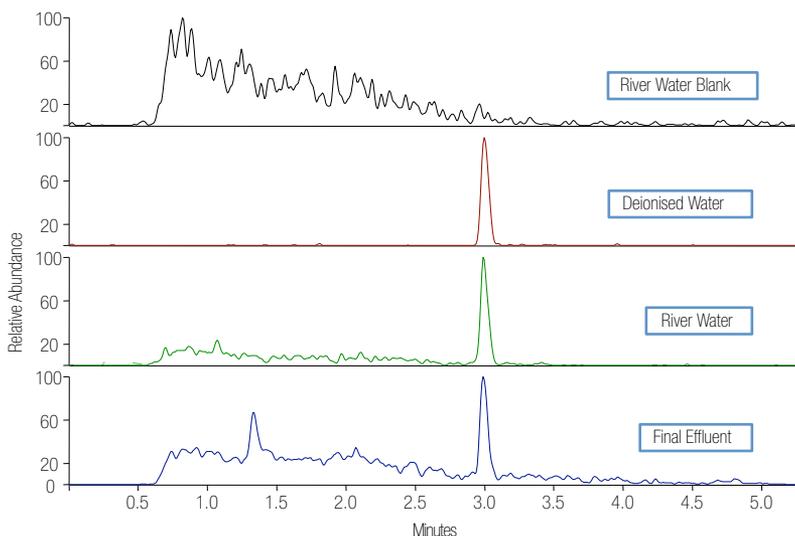
Group	LC system	Injection Volume (µL)	MS Analyzer (Acquisition mode)
Herbicides	Thermo Scientific™ UltiMate™ 3000 UHPLC	10 (offline) 100 (Large Vol Inj) 1000 (online*)	Thermo Scientific™ TSQ Endura™ Triple Quadrupole MS (SRM)
Insecticides	UltiMate 3000 UHPLC	10 (offline) 100 (Large Vol Inj) 1000 (online*)	TSQ Endura Triple Quadrupole MS (SRM)
Fungicides	UltiMate 3000 UHPLC	10 (offline) 100 (Large Vol Inj) 1000 (online*)	TSQ Endura Triple Quadrupole MS (SRM)
Pharmaceuticals	UltiMate 3000 UHPLC	20 (offline) 2000 (online*)	Thermo Scientific™ TSQ Quantiva™ Triple Quadrupole MS (SRM)
Endocrine Disruptors Hormones	UltiMate 3000 UHPLC	50 (offline) 2000 (online*)	TSQ Quantiva Triple Quadrupole MS (SRM)
Perfluorooctane sulfonic acid (PFOS)	UltiMate 3000 UHPLC	20 (offline) 2000 (online*)	TSQ Quantiva Triple Quadrupole MS (SRM)

\* EQuan MAX Plus LC-MS Systems

## Screening Solutions

The combination of both targeted and non-targeted analyses in a single run is realized with the Thermo Scientific™ Exactive™ Plus Orbitrap and Q Exactive™ Hybrid Quadrupole-Orbitrap high-resolution, accurate mass spectrometers.

- Built on proven Orbitrap technology
- Resolving power up to 140,000 FWHM (@ $m/z$  200)
- Easy separation of matrix from analytes for low LODs in complex environmental matrices
- Day-to-day robustness and mass accuracy stability
- Data-dependent MS/MS for screening, quantitation, and confirmation in one run



The analysis of 17β estradiol ( $m/z$  271>145) by LC-APCI-MS/MS in different environmental samples at a level of 350 pg/L (250 mL of sample extracted and 50 µL injection).

# Software Solutions

## Data Processing and Reporting—an integrated solution for your LC and GC analysis

Thermo Scientific™ TraceFinder™ software is a unique, workflow-oriented software for routine quantitation, targeted screening and qualitative review of data.

- Compatible with all Thermo Scientific quantitative GC and LC mass spectrometry platforms, to include non-mass spectrometer detectors, TraceFinder software offers one easy-to-use solution for all analytical laboratories.
- Designed to make routine quantitation and target analysis simple, fast, and productive. The software offers a simplified workflow-driven method setup with fully automated data acquisition, data processing and reporting.
- Advanced tools such as intelligent sequencing, custom report creation and high-resolution, accurate mass for screening.

Thermo Scientific™ Dionex™ Chromeleon™ 7.2 Chromatography Data System (CDS) software is the first CDS that combines separation (GC/IC/LC) and mass spectrometry (MS) in an enterprise environment. Chromeleon 7.2 Service Release 1 now provides control for Thermo Scientific LC-MS instruments. It offers:

- One software platform that streamlines chromatography and MS quantitation workflows, produces fewer analytical errors, and requires less training effort through built-in eWorkflows
- Productivity tools for instant data processing, accurate peak detection, and flexible spreadsheet-based reporting
- Future-proofed, scalable, and flexible architecture that lets you use your MS just like you would use other routine detectors



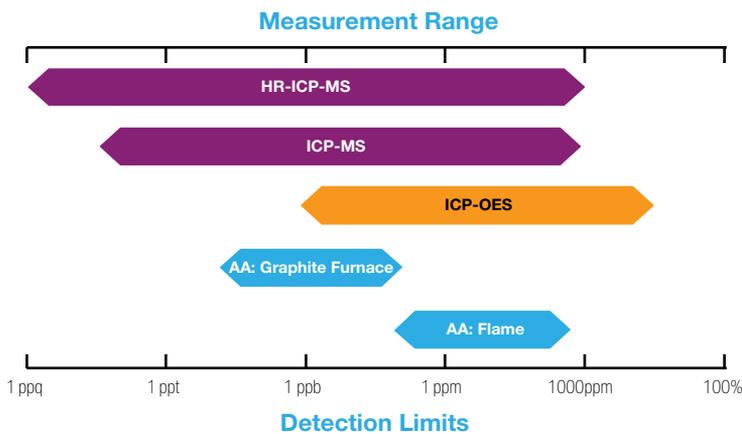
# Trace Elemental Analysis: Recommended Configurations

Element	Analyzer
Nickel	iCAP Q ICP-MS, iCE 3500 GF-AAS, or iCAP 7000 Series ICP-OES
Cadmium	ICAP Q ICP-MS, iCE 3500 GF-AAS
Mercury	ICP-MS, Vapor Generation" by: ICP-OES with hydride generation Vapor Generation" by: iCE series with hydride generation
Lead	Thermo Scientific™ ICAP™ Q ICP-MS, Thermo Scientific™ iCE™ 3500 GF-AAS

Sample preparation: Stabilization with nitric acid and dilution if required.

Selecting a technique to use in your laboratory for metals analysis in water requires consideration of these criteria:

## 1. Detection limits and measurement range 2. Analysis speed

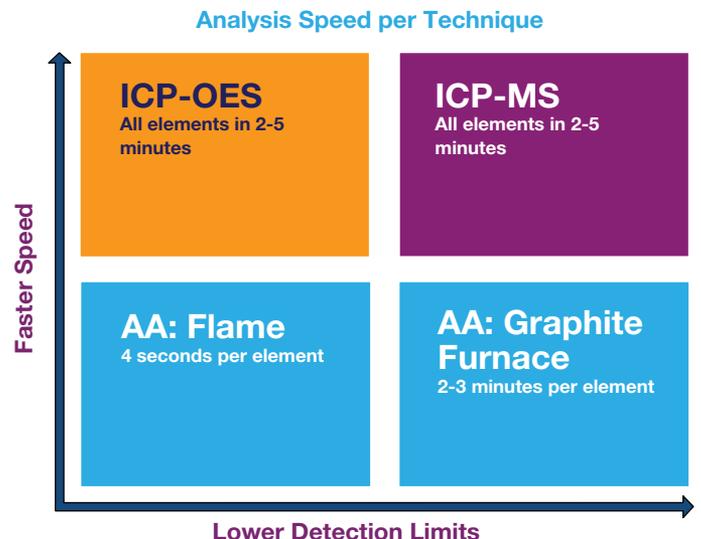


### 1. Detection Limits and Measurement Range

Consider the required detection limits for the metals you will need to analyze. Will one technique cover all the metals, or will you require multiple techniques?

### 2. Analysis Speed

Consider the analysis time for each technique, and the number of samples you will need to test in a day. Which technique will fit into your timelines? Does the same technique that supports your timeline also support the detection limits you require?



# One source, infinite solutions

Thermo Fisher Scientific has a complete portfolio of analytical solutions that will resolve your most challenging assays with reliability and confidence.

In addition to analytical instruments, we offer laboratory equipment, reagents, columns, consumables, and services to support our customers.

## Recommended references and resources

Heinz Singer et al. Determination of biocides and pesticides by on-line solid phase extraction coupled with mass spectrometry and their behavior in wastewater and surface water published at *Environmental Pollution* – 2010 (158) 3054-3064

Liza Viglino et al. On-line solid phase extraction and liquid chromatography/tandem mass spectrometry to quantify pharmaceuticals, pesticides and some metabolites in wastewaters, drinking and surface waters published at *Journal of Environmental Monitoring* – 2008 (10) 482-489

Laszlo Hollosi et al. Analytical sensitivity of direct injection LC-MS methods for the compounds of EU Water Frame Work directive presented at SETAC Glasgow 2013

Marina Gorga et al. Multi-residue analytical method for the determination of endocrine disruptors and related compounds in river and waste water using dual column liquid chromatography switching system coupled to mass spectrometry published at *Journal of Chromatography A* – 2013 (1295) 57-66

Rebeca López-Serna et al. Direct Analysis of pharmaceuticals, their metabolites and transformation products in environmental waters using on-line TurboFlow chromatography-liquid chromatography-tandem mass spectrometry published at *Journal of Chromatography A* – 2012 (1252) 115-129

Marta Llorca et al. Analysis of perfluoroalkyl substances in waters from Germany and Spain published at *Science of the Total Environment* – 2012 (431) 139-150

Sara Valsecchi et al. Optimisation of an on-line SPE-UHPLC/MS/MS method for the analysis of perfluoroalkylated acid in Italian drinking and surface waters presented at SETAC Glasgow 2013

Application note 52389 – Consolidated GC-MS/MS Analysis of OCPs, PAHs, and PCBs in Environmental Samples

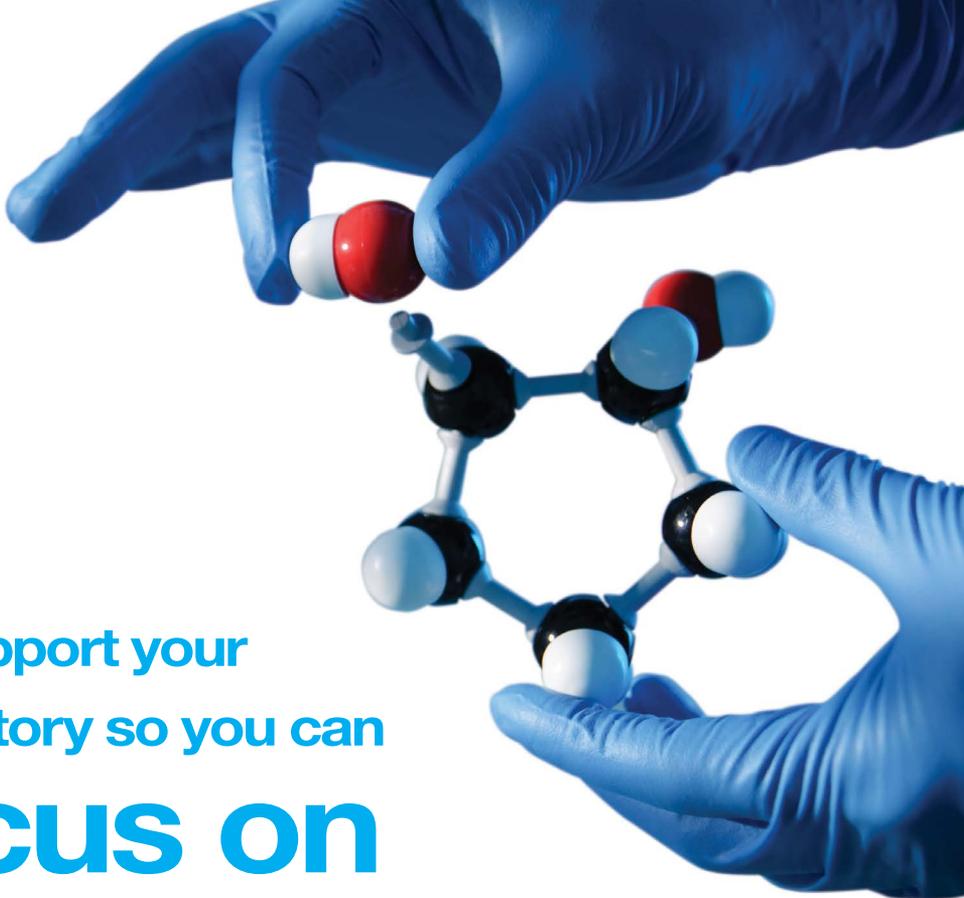
Technical Note 10319 – Simplifying Complex Multi-Residue Pesticide Methodology in GC-MS/MS

Technical Note 52099 – The Determination of Organotins in Water using Triple Quadrupole GC-MS/MS

Application Note 30098 – DFS- Analysis of Brominated Flame Retardants with High Resolution GC/MS

Application Note 43098 – Speciation analysis of Cr (III) and Cr (IV) in drinking waters using anion exchange chromatography coupled to the Thermo Scientific iCAP Q ICP-MS

Thermo Scientific application notes, technical notes, product information, videos, webinars, whitepapers, and other resources for water analysis are available at [www.thermoscientific.com/environmental-community](http://www.thermoscientific.com/environmental-community).



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the science**

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Let our expertise complement yours.

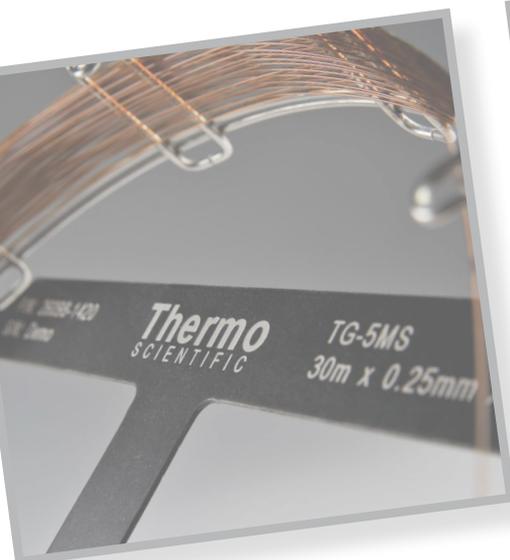
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