

# All Eyes on Environmental Analysis

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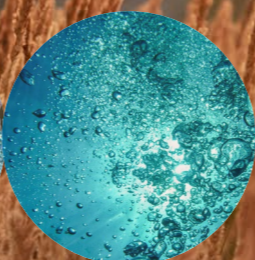
Online SPE for emerging contaminants



PFAS Analysis



LC-MS/MS analysis of polar pesticides



Hormones in your tap water?



PPCP's in water



LC-MS/MS for aqueous microcystins



Microplastics Analysis



# AUTOMATED ONLINE SPE-UHPLC/MS/MS ANALYSIS OF EMERGING POLLUTANTS IN WATER

Simultaneous quantification of contaminants  
in environmental water matrices

*Mengmeng Zhong, Tielong Wang, Jun Huang, and Gang Yu, School of Environment,  
Tsinghua University, Beijing, China. Meiling Lu, Agilent Technologies (China) Co. Ltd.*

In this application note, an automated online solid phase extraction (SPE) method coupled to ultrahigh-performance liquid chromatography/tandem mass spectrometry (UHPLC/MS/MS) is described for simultaneous determination of emerging organic contaminants (EOCs) in environmental water matrices. A total of 87 EOCs, including 58 pharmaceuticals and personal care products (PPCPs), 22 perfluoroalkyl substances (PFASs), and seven organophosphorous flame retardants (PFRs), were selected as the target analytes. Through optimization of the online SPE sample enrichment parameters and the LC/MS separation and detection conditions, the method was evaluated for performance across all 87 analytes in environmental water matrices including drinking water, surface water, and wastewater effluent. The optimized method delivered very good linearity, analytical sensitivity (LOQs <10 ng/L for almost all analytes), accuracy, and precision, and can be reliably applied for high-throughput screening of these EOCs in environmental water matrices.

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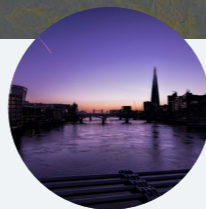


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# ANALYSIS OF >50 LEGACY AND EMERGING PFAS IN WATER USING THE AGILENT 6495B TRIPLE QUADRUPOLE LC/MS

*Timothy L Coggan, Jeff Shimeta, and Bradley O Clarke, RMIT University, Melbourne, VIC, Australia. Tarun Anumol and James Pyke, Agilent Technologies, Inc.*

The contamination of the environment with per- and polyfluoroalkyl substances (PFAS) is a serious concern to regulators, scientists, and the public worldwide due to their ubiquitous presence, persistence, and toxicity. Robust analytical techniques that can accurately and precisely quantify these pollutants at trace levels are necessary for understanding their environmental fate, ecological impacts, and impacts on public health. Appropriate analytical techniques and the fundamental data they generate allow scientists and regulators to make informed assessments of PFAS use in modern society.

This application note describes a sensitive and reliable method for the simultaneous quantitation of 53 legacy and emerging PFAS from 14 compound classes.

The method uses isotope dilution on an Agilent 1290 Infinity II LC coupled to an Agilent 6495B triple quadrupole LC/MS.

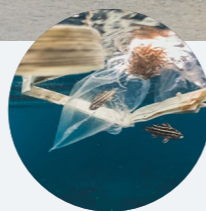
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# MEASUREMENT OF UNDERIVATIZED GLYPHOSATE AND OTHER POLAR PESTICIDES IN SURFACE AND DRINKING WATER

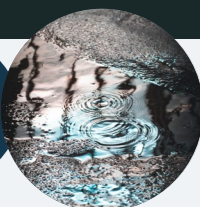
Using reversed-phase chromatography and tandem mass spectrometry

*Jean-Francois Roy, Jarod N Grossman, and Tarun Anumol, Agilent Technologies, Inc.*

The accurate quantitation of glyphosate and other highly polar pesticides at nanogram per liter (ng/L) levels in surface and drinking water has proven to be challenging, given the polar nature of these compounds. A simple yet effective methodology involving liquid chromatography coupled to tandem mass spectrometry (LC/TQ) is presented here. The method includes quick and effective sample preparation without derivatization, robust reversed-phase chromatography, and extremely sensitive mass spectrometry detection for routine analysis.

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# MASS SPECTROMETRY ANALYSIS OF HORMONES IN WATER BY DIRECT INJECTION

Using the Agilent 6470 Triple Quadrupole Mass Spectrometer

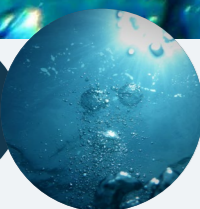
*Imma Ferrer, E Michael Thurman, and Jerry A Zweigenbaum,  
University of Colorado and Agilent Technologies, Inc.*

Some hormones are included in the Contaminant Candidate List CCL4 of the Environmental Protection Agency (EPA) to be assessed for regulation in drinking water. These compounds are also of regulatory interest in the EU, China, and other countries. Therefore, the environmental community often desires the analysis of these compounds in water samples. This Application Note describes the methodology used for the determination of eight hormones (17- $\alpha$ -ethinylestradiol, 17- $\beta$ -estradiol, estriol, 4-androstene-3,17-dione, equilin, estrone, progesterone, and testosterone) in tap water using an Agilent 6470 triple quadrupole mass spectrometer. A direct injection method using 100  $\mu$ L of water sample was carried out. This method saves time, reduces handling errors and analytical variability, and is sensitive enough to detect hormones in surface and drinking water at ng/L levels.

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# ANALYSIS OF WASTEWATER EFFLUENT SAMPLES TO IDENTIFY TOXIC CHEMICALS USING THE HIGH-RESOLUTION AGILENT 7250 GC/Q-TOF

*Sofia Nieto and Kai Chen, Agilent Technologies, Inc. Thomas Young,  
Department of Civil and Environmental Engineering,  
University of California Davis, CA, USA*

This study used a workflow for broad scope suspect screening to identify toxic chemicals in wastewater effluents. The comprehensive approach combined targeted and untargeted methods using a high-resolution accurate mass Agilent 7250 GC/Q-TOF in multiple ionization modes, the GC/Q-TOF screening workflow in Agilent MassHunter Quantitative Analysis software 10.1, and the GC/Q-TOF accurate mass library of pesticides and environmental contaminants.

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# QUANTITATION OF MICROCYSTINS IN WATER BY DIRECT INJECTION AND ONLINE SPE LC/MS/MS SYSTEMS

Chang jiang, Pei-bin Hu, Agilent Technologies Inc., Chengdu, China.  
Tarun Anumol, Agilent Technologies Inc., Wilmington, DE, USA

This application note compares direct injection and online SPE methods using liquid chromatography (LC) coupled with tandem mass spectrometry (MS/MS) to analyze microcystins (MCs) in water. These include MC-RR, MC-HtyR, MC-LR, MC-HilR, MC-LA, and MC-LF. The online SPE LC/MS/MS system eliminates time-consuming and laborious offline SPE extraction steps. Both the direct injection and online SPE method achieved limits of detection (LODs) of low or sub-ng/L levels, which are much lower than the provisional guidelines for drinking water expressed by the World Health Organization (WHO).

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# FAST, AUTOMATED MICROPLASTICS ANALYSIS USING LASER DIRECT CHEMICAL IMAGING

Characterizing and quantifying microplastics  
in water samples from marine environments

*Lars Hildebrandt, Fadi El Gareb, Tristan Zimmermann, Ole Klein, Kay-Christian Emeis and Daniel Proefrock, Institute of Coastal Research, Helmholtz-Zentrum Geesthacht, Germany.  
Andreas Kerstan, Agilent Technologies, Inc.*

It is estimated that more than 75% of the 8.3 billion metric tons of plastic produced over the last 65 years have turned into waste. Up to 13 million metric tons of this waste ends up in the ocean every year and recent calculations estimate that more than 5.25 trillion plastic particles float in the world's oceans.

Scientists have demonstrated the alarming environmental ubiquity and persistence of particulate plastic in aquatic ecosystems. Models predict that approximately 14% of the plastic debris in the ocean surface layer can be classified as so-called microplastics (often referred to as particles between 1  $\mu\text{m}$  and 5 mm in size). These ingestible and potentially harmful particles have been formed by UV-induced, mechanical, or biological degradation of larger debris items. To verify the estimates and to meet upcoming regulatory measures (e.g., California Senate Bill 1422) and directives (MSFD, 2008/56/EC), accurate, time-efficient, and robust analytical workflows and techniques are required. Learn how Laser Direct InfraRed (LDIR) Chemical Imaging Spectroscopy is used to achieve this goal.

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