

# The Measure of Purity

Water quality applications



# Safeguarding a Precious Resource

Of all our planet's natural resources, none is more essential to life than water. Unfortunately, this precious resource is both limited and in jeopardy. Clean water sources are running dry, chemical contamination threatens existing supplies, and emerging hazards are being identified every year.

To ensure water safety—and to protect human health—governments and private institutions continuously monitor water quality, and establish regulations to protect essential water sources.

Agilent supports water testing success by providing reliable, high-productivity tools. These include robust detectors, workflow solutions for organic and inorganic analysis, and strategies for minimizing matrix interference. So you can achieve the selectivity and low limits of detection (LOD) you need to be certain that water quality meets regulatory standards.



# Agilent water quality solutions extend across all chemical classes

For more than 40 years, Agilent has been helping our customers safeguard the world's water supply. How? By combining an expanded analytical portfolio with unrivaled leadership in water quality measurement.

We will continue to offer the most accurate, sensitive, and reliable solutions to meet ever-changing water testing and analysis requirements.

# Volatiles Measurement

Maximize productivity, sensitivity, and reliability



Volatile organic compounds (VOCs) enter our water supply in various ways. Industrial processes, biological contamination, and water disinfection treatments all produce VOCs that can lead to cancer, organ damage, and disease. To reduce the risks associated with these compounds, many governments closely regulate the amounts that are allowed in drinking water.

By combining robust instruments and columns with innovative features that maximize throughput, Agilent equips you for high-productivity measurement of VOCs in water.

### High-capacity headspace sampling

Simple headspace extraction is ideal for volatiles in water because it transfers less water to the GC and has few parameters to adjust. During headspace sampling, vials are heated (and may be treated with salt) to force volatile compounds into the headspace above the sample. The headspace is then sampled, and an aliquot is delivered to the GC.

When used with selected ion monitoring (SIM) mode in a mass spectrometer, headspace sampling can achieve parts-per-trillion (ppt) levels of volatile contaminant detection.

The Agilent 7697A headspace sampler features high sample capacity and built-in electronic pneumatic control (EPC) to maximize performance over a wide concentration range. Its inert sample pathway prevents analyte degradation or loss, so you can achieve limits of quantitation lower than US EPA regulations and EU directives.



**Agilent 8890 GC/MSD with 7697A headspace sampler.** Headspace sampling ensures an inert sample pathway for superior GC/MSD performance without analyte degradation or loss.

### GC/MS analysis of drinking water

In this example, we used the Agilent 7697A headspace sampler, followed by separation and detection with an Agilent GC/MSD single quadrupole system. The GC/MSD was operated in simultaneous SIM/SCAN mode with the trace ion detection mode switched on.

This application meets EU requirements for volatiles in water as outlined in 98/83/EC Directive. Calibration from 0.05 to 20 ppb showed excellent % relative standard deviations (RSDs) and linearity for all analytes. Reproducibility of replicate injections resulted in instrument detection limits <0.10 ppb for all 60 compounds.

Export MSD ChemStation Quant Database	? ×
Qptions	
Input MSD ChemStation Quant Database	
D:\from Mikesys\MSDChem\methods-2\VOA-HS_DA.m\qdb.mth	Browse
Output MassHunter Quantitation Method	
voa.quantmethod.xml	Choose Folder
Betrand Standard Compounds  Detricolificamentariae  Oricomethane  World Cloade  Bonnorethane  Torothane  Torothanethane  Torothanethanethanethanethanethanethanethane	<
- 1,2-Dichloroethene (cis) - 2,2-Dichloropropane	-
Export to MassHunter Quantitation Method	
MassHunter GC/MS Translator B.06.00 1116 10-Apr-2012 Translation was suc	cessful.

Agilent MassHunter 5977 data analysis. You can easily convert existing MSD ChemStation data analysis methods to MassHunter methods.



**Agilent MassHunter data analysis software.** Vinyl chloride calibration from 0.10 to 40 ppb. [5991-2108EN: *Environmental VOCs Using an Agilent Headspace Sampler with 7890B GC/5977A GC/MSD*]

### Sensitive purge and trap autosampling

Agilent purge and trap (P&T) instruments combine highsensitivity VOC detection with low carryover—giving you ultimate confidence in sample-to-sample measurement.

- Teledyne Tekmar Lumin P&T concentrator (PTC): A sample preparation instrument that uses helium or nitrogen to remove VOCs from aqueous and solid samples.
- Teledyne Tekmar AQUATek LVA autosampler: A P&T autosampler that automates sample preparation steps for liquid sample analysis. Ideal for samples such as drinking water and wastewater.
- Teledyne Tekmar Atomx XYZ automated VOC sample preparation system: A single instrument that combines an autosampler with P&T, making it ideal for analyzing VOCs in soils and waters. It's also the only system that employs methanol extraction automation for high-level soils per US EPA Method 5035.

# Optimized VOC analysis in drinking water using purge and trap

The chromatogram on page 6 represents the analysis of volatiles in drinking water according to US EPA Method 524.2. We used the Teledyne Tekmar Atomx sample preparation system, combined with an Agilent 7890/5977B GC/MSD system.

In addition, the Agilent VOC applications kit (p/n G7022A) used for this analysis was optimized for:

- Speed. Analysis of 71 compounds was reduced to 15 minutes with the use of the 0.18 mm DB-624 UI column.
- Sensitivity. Limits of detection for high-performance P&T GC/MSD systems are typically in the low ppt range—and sometimes approach parts-perquadrillion (ppq).
- Resolution. The Ultra Inert column, liner, and El ion source provided stability, robustness, and excellent peak resolution.

A calibration curve ranging from 0.25 to 50  $\mu$ g/L routinely produced VOC average response factors of less than 20% relative standard deviation (RSD).





Atomx XYZ system and AQUATek LVA autosampler with Lumin P&T concentrator.



### System control and monitoring: VOC TekLink software

Once activated, VOC TekLink software continuously monitors your system to make sure that operating limits are not exceeded. The software also performs useful diagnostics, such as leak and benchmark tests for instrument validation. All instrument parameters, method scheduling, and editing can be programmed.

In addition, predeveloped methods are provided for easy start-up with little or no modification. An optional 21 CFR Part 11 data audit trail package is also available.

i 🖌 🔘 qe soi	YC	) ocw	ater 🗖 Aton	nse QC 🔲	bake			lool					×	Instrument Status		
17 💌 🗆	Dele	ste after	the next archive											Node:		
	To	add line	s to the schedule.	click anywhe	ere on t	he last li	ne and pre	ss the I	own arror	e keno.				Purge Ready		
··· 🗸	17	pe "0" fo	r a blank vial. To	insert blanks	every o	ther ne	w line, hold	Orlw	ile you pre	iss Down.				Load a schedule to begin		
	Use?	Vial	Method	Туре	STD 1	STD	2 STD 3	Dik	tion P	urge Be	ke p	Posn	Status	Schedule		
1	7	BLK	QC Water	Water	5	5	• S •	10	-					Schedule 555 has completed.	4-1-5	
2	4	2	QC Water	Water	0 .	0		1:1	-					Total kun Time: 1 hour(s) 45.2 min	ara(s)	-
3	1	3	QC Water	water	5 5	9.5		10	-					Click here to confirm and clear	E.	
2	1	1	QC water	water	0 1	9		10	-					Active Nethod: OC Water		
6		6	OC Water	Water	5			10	-					Zones		
7	R	RK	OC Water	Water	5 4	1.5		10	1					Name	Current	Set Point
8	7	8	OC Water	Water	5 4	1 5		1:10	0					Mass Flow	10 mL/min	10 mL/min
9	1	9	OC Water	Water	5 .	1 5	- 5 -	1.1						Pressure	0.8 psig	n/a
10	7	10	QC Water	Water	5 .	5	- 5 -	14						Svringe	0.0 ml	0.0 ml
11	7	11	QC Sol	Sol	5	5	• 5 •	10						Transfer Line	14190	140%
12	7	12	QC Sol	Sol	5	5	- 5 -	10						Ourse Line	14190	14090
13	7	13	QC Sol	Sol	5	5	• 5 •	10	×					Oven	141-0	140-0
14	7	14	QC Sol	Sol	5 .	5	- 5 -	1:	-					Mount	91°C	90°C
15	2	15	QC Sol	Sol	5	5	• 5 •	10	-					Trap	26°C	Ambient
16	4	16	QC Sol	Sol	5 .	5	- 5 -	1:3	-					Sample Vial	23°C	Ambient
1/	14	1/	QC MBOH	mechanor	5	5		115	0 🔟					Condensor	26°C	Ambient 🦱
10	14	10	QC Water	Water	0.0	9.		10						Soil Valve	9990	100%
20	1	19	OC Water	Water	5 .	1 5	. 5 .	10	-					Water	9200	90%
	100		40.000						<u>لنہ</u>					water	92 C	50 C

**Schedule screen** shows multiple methods, multiple internal standards, and various dilutions that can all be run on a single schedule. Schedules can be updated in real time.

#### **Status section**

This section shows the active mode, along with the time remaining for that mode.

#### **Zone section**

This section monitors actual values compared to method-driven setpoints.

## Semivolatiles and Pesticides Measurement

High performance, rugged dependability



Semivolatile organic compounds and pesticides can remain in the environment for a long time, presenting a constant threat to our water supply. Like VOCs, semivolatiles and pesticides may cause long-term health effects, and are regulated worldwide. They can also be tough to accurately quantify—especially when present in low concentrations.

### GC/MS solutions for pesticides

### Maintaining sensitivity and inertness despite matrix interference

Agilent mass spectrometers are known for their robustness, as well as their sensitivity in the ppb and ppt range. You also benefit from these leading-edge technologies:

- Deconvolution reporting software (DRS) reduces the impact of matrix interference through robust algorithms that deconvolute overlapping spectra. So you can increase the sensitivity of semivolatile and pesticide detection.
- Retention time locking (RTL) software reproduces retention times within fractions of a second from one Agilent GC system to another. That means you can reproduce results across instruments in your lab. The benefits are twofold: increased throughput and greater confidence in your results.
- Multimode inlet (MMI) is a programmable temperature-vaporizing inlet that can increase signal-to-noise ratios in cold splitless mode.
- Capillary flow technology (CFT) takes the complexity out of column backflushing for improved analytical results and increased sample throughput.
- Flexible comprehensive multiple reaction monitoring (MRM) database saves you time when creating GC/TQ pesticide methods. It contains MRM transitions and retention times for over 1,100 pesticides and pollutants.
- Analyzer solutions are preconfigured and chemically tested, helping you accurately confirm target analytes in complex matrices.



Together, the Agilent **8890 GC**, **5977B GC/MSD**, and **7693A automatic liquid sampler** quickly screen and quantitate large numbers of pesticides in a single analysis. Screening methods conform to the latest worldwide testing requirements.



The **Agilent 7000 Series GC/TQ** reduces or eliminates interferences that negatively impact accuracy and detection limits in traditional GC/MS SIM methods.

### Agilent 7000D triple quadrupole GC/MS

#### Perform sensitive, multiresidue analyses in complex matrices

High-boiling molecules that flood out of the GC column after separation can reduce GC/MS/MS reliability for complex matrices, and force extra maintenance.

The Agilent 7000D triple quadrupole GC/MS system is the only MS/MS analyzer designed to operate at temperatures as high as 200 °C. Because the quadrupole can be kept at higher temperatures, and at vacuum, it stays clean even with complex, high-boiling samples. This minimizes time-consuming maintenance and improves mass analyzer performance.

In this example, eight polycyclic aromatic hydrocarbons (PAHs) and six polybrominated diphenyl ethers (PBDEs) were extracted from wastewater with no cleanup. They were then analyzed on the 7000D triple quadrupole GC/MS. The desired detection was achieved with 25  $\mu$ L injections using the Agilent MMI in solvent vent mode. Labeled analogues were used as internal standards for each compound of interest.



Start 2 Crog- Feet

A screen capture of **Agilent MassHunter quantitative software** displays the batch table of the 26 samples analyzed in the sequence. Extracted ion chromatograms for PBDE 47 and its internal standard (13C PBDE 47) show a distinct peak above baseline, even at 2 ppt. The calibration curve of the PBDE 47 is displayed between 0 and 10 ppt.



This 20-minute chromatogram demonstrates the separation of PAHs and PBDEs. Labeled analogues were used as internal standards for each compound of interest.

This list shows eight PAHs identified by the EPA as possible human carcinogens. It also shows six PBDEs that are halogenated flame-retardant chemicals. These compounds are used in products such as textiles, plastics, wire insulation, and automobiles.

The EPA is concerned that certain PBDE congeners may be persistent, bioaccumulative, and toxic to people and the environment.

#### Compounds (Limit of Detection in $\mu$ g/L)

naphthalene	(2.0)	benzo[g,h,i]perylene	(0.001)	
anthracene	(0.1)	polybrominated diphenyl ether	(PBDE) 28	
fluoranthene	(0.1)	polybrominated diphenyl ether	(PBDE) 47	( <b>-</b> )
benzo[b]fluoranthene	(0.015)	polybrominated diphenyl ether	(PBDE) 99	(0.0005) total
benzo[k]fluoranthene	(0.015)	polybrominated diphenyl ether	(PBDE) 100	
benzo[a]pyrene	(0.05)	polybrominated diphenyl ether	(PBDE) 153	
indeno[1,2,3-cd]pyrene	(0.001)	polybrominated diphenyl ether	(PBDE) 154	

Detection limits were met for all compounds from 2 ppb to less than 0.5 ppt. The run took place in less than 20 minutes with simple liquid—liquid sample preparation (hexane extraction), no sample cleanup, no solvent switching, and all 14 analytes present. [5991-0017EN: *Analyzing Wastewaters for PAHs and PBDEs Using the Agilent 7000 Triple Quadrupole GC/MS*]

### LC/MS analysis of pesticides

#### Agilent InfinityLab Online SPE Solutions

Whether you need to enrich your analytes, remove matrix components, or lower detection limits, Agilent InfinityLab Online SPE Solutions are a flexible choice. Their modular design lets you tailor your system to match virtually any analytical challenge.

Agilent InfinityLab Online SPE Solutions are based on the 1290 Infinity Flexible Cube, coupled with a 6400 Series triple quadrupole LC/MS system. The 1290 Infinity Flexible Cube houses reusable SPE cartridges and up to two valves, allowing rapid, automated extraction and analysis of water samples. In addition, Agilent InfinityLab Quick Change valves let you easily mount your valve heads on the valve drives. The sample is flushed onto the cartridges using a loading pump.

An extensive portfolio of valves makes it easy to customize your InfinityLab Online SPE System to fit your needs. Combine these kits with the Online SPE Starter Set for applications such as:

- Direct injection
- Multi-cartridge kit
- High-volume injection

The high precision and accuracy of the Agilent InfinityLab Online SPE Solutions could be demonstrated in the analysis of herbicides at trace levels down to 1 ng/L (LOQ) in drinking water.

#### Quantify trace-level herbicides in drinking water

We demonstrate the high precision and accuracy of Agilent InfinityLab Online SPE Solutions in this analysis of herbicides at trace levels down to 1 ng/L (LOQs).

Compound	LOQ (ng/L)	LOD (ng/L)	Recovery (%)
Atrazine desisopropyl	5	2.0	84.3
Carbendazim	1	0.5	88.8
Metamitron	5	2.0	87.8
Fenuron	2	1.0	96.1
Atrazine desethyl	5	2.0	92.2
Chloridazon	2	1.0	96.8
Carbetamide	2	1.0	98.5
Metoxuron	2	1.0	96.8
Monuron	2	1.0	97.0
Simazine	5	2.0	97.9
Cyanazine	5	2.0	92.0
Methabenzthiazuron	1	0.5	95.5
Chlorotoluron	1	0.5	94.9
Desmetryn	1	0.5	95.6
Atrazine	2	1.0	96.9
Isoproturon	1	0.5	98.0
Diuron	2	1.0	82.1
Monolinuron	5	2.0	92.3
Propazine	2	1.0	94.6
Linuron	5	2.0	87.1
Terbuthylazine	1	0.5	100.9
Chloroxuron	1	0.5	105.5
Irgarol 1051	1	0.5	89.8
Pormetryn	1	2.0	94.3
Diflubenzuron	5	2.0	78.0
Terbutryn	1	0.5	97.4
Trietazine	5	2.0	97.3

Performance data of all herbicides, showing limits of quantification (LOQ, S/N = 10), limits of detection (LOD, S/N = 3), and recovery in a spiked water sample. [5991-1738EN: Quantification of Trace-Level Herbicides in Drinking Water by Online Enrichment With the Agilent 1200 Infinity Series Online Spe Solution and Triple Quadrupole MS Detection].



Agilent InfinityLab Online SPE Solutions

The Agilent pesticide-triggered MRM (tMRM) LC/MS application kit completes most of the development work for you. It features easy-to-use examples that demonstrate how to set up screening methods and quickly adapt them to your needs.

You'll also benefit from:

- A tMRM database and library for more than 700 pesticides. The library includes compound names, up to 10 MRM transitions, fragmentor voltages, collision energies, and the ability to add retention times for each compound. So you can reliably screen pesticides with tMRM library verification.
- Pretested analysis methods, using the tMRM database, for target screening of pesticides routinely monitored around the world.



MRM chromatograms for a calibration standard with a concentration of 100 ppt (ng/L). Each of the 28 pesticides in the Online SPE method were measured in dynamic MRM mode with a quantifier and qualifier ion.



Total ion MRM chromatogram of  $0.5 \mu g/L$  standard of acidic herbicides. [5990-4864EN: Determination of Acidic Herbicides Using an Agilent 6460 Triple Quadrupole LC/MS Equipped with Agilent Jet Stream Technology and Direct Aqueous Injection, for Potable and Environmental Samples]

# Emerging Contaminants Measurement

Sensitive detection and identification for knowns and unknowns



Pharmaceutical and personal care products (PPCPs), perfluorinated alkyl substances (PFAS), and endocrine disruptors have been identified as chemical threats to our water supplies. While many of these compounds are not yet regulated, they have been subjected to increased scrutiny—and the list of monitored compounds grows every year.

Agilent helps you monitor known emerging contaminants, and identify unknown emerging threats. Our LC/MS and GC/MS systems provide sensitive detection and identification of diverse trace analytes.

## Triple quadrupole LC/MS

### Detect hundreds of trace-level polar compounds per injection

The high polarity and low levels of many PPCP and PFAS contaminants make LC/MS analysis the method of choice. Together, the Agilent 6400 triple quadrupole LC/MS and 1290 Infinity II LC System provide fast, multi-analyte quantitation. You also get the benefits of MRM at low ng/L levels in water samples.

In addition, the revolutionary Agilent Ultivo triple quadrupole LC/MS is the only fully stackable system that saves you bench space without sacrificing sensitivity or reliability. It is ideal for analysis of regulated and emerging contaminants in water.



The Agilent 6400 triple quadrupole LC/MS and 1290 Infinity II LC System meet your needs for target compound analysis.

#### Sensitive, accurate screening of target PPCPs and PFASs

The unmatched sensitivity and fast MRM switching speeds make Agilent 6400 Series triple quadrupole systems ideal analytical tools.



We confirmed the presence of two PPCPs in surface water by direct aqueous injection into the Agilent 6400 Series LC/MS. The qualifying ion abundances for these compounds are also shown. Both pharmaceuticals (diltiazem and sulfamethoxazole) were readily identified and quantitated in this complex matrix due to MRM transition selectivity and instrument sensitivity. [5990-6431EN: Direct Aqueous Analysis of Pharmaceuticals in Water at ppt Levels by LC/MS/MS with Agilent 6490 Triple Quadrupole LC/MS System with Ion Funnel Technology]

# Low limits of detection: analysis of drinking water

Here, PFAS on US EPA and EU monitoring lists were screened at lowlevel pg on-column in a potable water matrix. We achieved zero background interference using dynamic MRM. This approach allowed us to gain reliable, positive identifications and low limits of detection.

Name	Compound Group	RT	R <sup>2</sup>	6470 IDL (pg)	EPA LOD (pg on-column)	Precision at 1.6 pg on-column, FTA-e at 31 pg on-column (%)
PFBA	Acid	4.11	1.000	0.025		4
PFPeA	Acid	7.17	1.000	0.025		5
PFHxA	Acid	9.26	0.998	0.025	4.00	5
PFHpA	Acid	10.72	0.999	0.025	1.25	7
PFOA	Acid	11.83	0.997	0.200	4.25	3
PFNA	Acid	12.74	1.000	0.100	1.75	8
PFDA	Acid	13.51	0.999	0.100	1.75	6
PFUdA	Acid	14.16	0.997	0.200	7.00	6
PFDoA	Acid	14.73	0.996	0.200	2.75	10
PFTrDA	Acid	15.22	0.999	0.025	5.50	8
PFTeDA	Acid	15.65	0.999	0.050	4.25	6
FOSA	FOSA	14.08	1.000	0.025		8
N-MeFOSAA	FOSAA	13.85	0.992	0.100	16.25	4
N-EtFOSAA	FOSAA	14.18	0.999	0.050	10.50	7
FHEA	FTA-e	11.06	1.000	16.000		7
FOEA	FTA-e	13.04	0.999	8.000		9
FDEA	FTA-e	14.43	0.996	16.000		15
PFHpPA	FTA-p	12.98	1.000	0.200		4
4-2 FTS	FTS	9.12	0.998	0.200		7
6-2 FTS	FTS	11.78	0.996	0.200		9
8-2 FTS	FTS	13.50	0.994	0.400		14
6-2 FTUA	FTUA	10.99	0.999	0.025		5
8-2 FTUA	FTUA	12.99	0.999	0.025		8
PFBS	Sulfonate	7.77	1.000	0.025	7.75	4
PFPeS	Sulfonate	9.53	0.998	0.025		6
PFHxS	Sulfonate	10.83	0.999	0.025	5.00	4
PFHpS	Sulfonate	11.88	0.999	0.025		7
PFOS	Sulfonate	12.75	0.999	0.025	3.50	8
PFNS	Sulfonate	13.49	0.993	0.200		11
PFDS	Sulfonate	14.13	0.994	0.100		4



All compounds 20 ng/L equivalent (25 pg on-column), except FTA-e, at 400 ng/L equivalent (500 pg on-column).

### GC and LC/Q-TOF:

#### Unambiguously determine the structure of unknowns

With sub-ppm mass accuracy and ultrahigh resolution, Agilent GC and LC/Q-TOF systems help you reduce uncertainty and minimize false positives. They also let you improve database search scores and generate molecular formulas for identification of unknowns.

What's more, enhanced resolving power and isotopic fidelity let you reliably detect mass peaks of interest. A dynamic range of up to five orders in-spectrum uncovers low-abundance compounds in the presence of higherabundance components. So you can reliably identify compounds in water samples, and completely characterize chemical contamination.



Agilent 7250 GC/Q-TOF with 8890 GC/MS.



Agilent 1290 Infinity II LC System and 6500 Series accurate-mass quadrupole time-of-flight (Q-TOF) LC/MS.







EIC of an unexpected contaminant, metoprolol, with a signal-tonoise ratio of 46:1. Red squares represent the theoretical isotope intensity and position.

# Inorganic and Elemental Analysis

Detect potentially harmful levels of trace and minor elements



Inorganic elemental contamination of water supplies may occur from natural deposits as well as from industrial, agricultural, and household sources.

Monitoring these contaminants in fresh water sources is essential to protecting human health. However, it can be challenging to monitor metals in diverse samples, where quantities can range from trace levels to high concentrations.

Agilent instruments deliver sensitive, accurate, and precise measurements across a wide dynamic range, from percentage to low ng/L, and in the presence of matrix interference. Each instrument has unique performance characteristics, so you can choose the technique that meets your analytical needs and your requirements for sample matrix, throughput, and budget.

This table will help you select the right Agilent instrument for robust, sensitive detection.

Criteria	Flame AA	GFAA	MP-AES	ICP-0ES	ICP-MS
Measurement range					
> 10%				•	
1-10%	•		•	•	
1–10,000 ppm	•		•	•	•
100-1,000 ppb	•	•	•	•	•
1–100 ppb		•	•	•	•
ppt		•			•
<ppt< td=""><td></td><td></td><td></td><td></td><td>•</td></ppt<>					•
Number of samples					
Few	•	•	•	•	•
Several	•		•	•	•
Many				•	•
Number of elements per sample					
Single/few (1-5)	•	•	•	•	•
Intermediate (5-10)	•		•	•	•
Many				•	•
Sample matrix					
< 3% solids	•	•	•	•	•
3-10%*	•	•		•	•
> 10%		•		•	
Advanced applications					
Chromatographic coupling					•
Nanoparticle characterization					•
Isotopic analysis/IDMS					•

\*Agilent ICP-MS systems with UHMI tolerate up to 25% total dissolved solids (HMI up to 3% TDS).

### **Atomic absorption**

#### Detecting trace metals in water

Agilent 280Z Zeeman graphite furnace AA spectrometers (GFAAS) deliver greater sensitivity with extended tube lifetimes. That makes GFAA a suitable alternative for analyzing heavy metals on a limited budget, or as a backup to ICP-OES.

Mercury is one of the most toxic heavy metals. US EPA Method 245.1 is the approved method for determining mercury in industrial effluents—as well as drinking, surface, ground, sea, and brackish waters. The method relies on cold vapor AA with stannous chloride as the reducing agent.

Element	MDL (µg/L)	Element	MDL (µg/L)
As	0.5	Ni	0.6
Ве	0.02	Pb	0.7
Cd	0.05	Sb	0.8
Со	0.7	Se	0.6
Cr	0.1	Sn	1.7
Cu	0.7	TI	0.7

This table lists the detection limits of the Agilent 280Z GFAAS for a range of common elements per US EPA Method 200.9: Trace Elements in Water, Solids, and Biosolids by Stabilized Temperature GFAAS.

Combining the Agilent VGA 77 vapor generation accessory with the 240 Series AA offers several advantages for this method:

- High sample throughput and full automation capabilities.
- Precise, accurate results with a Hg detection limit of 0.05 µg/L. Precision is typically better than 1% at the 2 to 3 µg/L level, achieving excellent accuracy.

Reference Standard	Measured Value (µg/L)	Certified Value (µg/L)	Valid Range	% Recovery
Hg 1	0.46	0.42	na	110
Hg 2	2.44	2.4	na	102
Hg 3	7.28	7	na	104
WS 2	1.88	1.8	1.4-2.2	104
WS 13	1.51	1.4	1.0-1.7	108
TM 1	0.74	0.7	0.3-1.1	106
TM 2	8.94	8.7	5.9-11.1	103
EP 1	49.9	50	na	100
EP 2	325	300	na	108

Correlation for mercury results between cold vapor AA determinations and certified values. The recoveries are all within +/- 10% of the expected value.



Agilent 7800 ICP-MS combines automated setup, fast analysis, and comprehensive interference removal. It also includes a simple hardware and software package.



Agilent 5110 SVDV ICP-OES provides the fastest, most precise inorganic analysis.



Agilent 4210 MP-AES performs multielement determination in water using plasma that runs on air for the lowest cost of ownership.



Agilent 280Z Zeeman is built for very low detection limits (low ppb or ppt).

### **ICP-OES** analysis

#### High volume, high productivity

ICP-OES is commonly used for water analysis around the world. Agilent ICP-OES systems offer the finest performance, productivity, and flexibility—making them ideal for determining trace and toxic elements in water.

The Agilent 5110 SVDV ICP-OES has a vertically oriented torch, plus optics that can take axial and radial measurements at the same time. This unique technology enables high-speed analysis, as well as robustness and sensitivity for complex matrix samples.

To test the capabilities of the 5110 ICP-OES, we determined 26 analytes in a certified reference water sample (CRM-TMDW-A). The following table confirms excellent agreement with the certified results as shown by % recovery.

#### Results for Determining 26 Analytes in a Certified Reference Water Sample

Note the excellent agreement with certified values for all analytes, demonstrating the accuracy made possible by the Agilent 5110 ICP-OES.

		CRM-TMDW-A		
Element/Wavelength (nm)	Certified (µg/L)	Measured (µg/L)	SD	Recovery (%)
Al 308.215	125	131.0	15.7	105
Sb 206.834	55	55.7	1.7	101
As 188.980	55	58.0	2.3	105
Ba 493.409	500	493.9	6.8	99
Be 313.042	15	15.0	0.4	100
B 249.772	150	152.4	0.8	102
Cd 226.502	10	10.0	0.4	100
Ca 315.887	31000	31573	423	102
Cr 205.552	20	20.2	0.3	101
Co 228.616	25	23.9	0.5	96
Cu 324.754	20	18.8	0.1	94
Fe 259.940	90	98.0	6.4	109
Pb 220.353	20	20.4	1.0	102
Li 670.784	15	13.5	0.3	90
Mg 279.079	8000	8175	54.8	102
Mn 257.610	40	39.5	1.1	99
Mo 203.846	110	110.5	1.4	100
Ni 231.604	60	64.5	3.6	108
K 766.491	2500	2563	19.6	103
Se 196.026	11	11.3	1.3	103
Ag 328.068	2	1.9	0.2	94
Na 589.592	2300	2412	24.9	105
Sr 421.552	300	308.1	5.1	103
TI 190.794	10	10.2	2.0	102
V 292.401	35	34.7	0.4	99
Zn 213.857	75	78.8	0.4	105

CRM-TMDW-A. [5991-4821EN: Ultra-fast ICP-OES Determination of Trace Elements in Water, Conforming to US EPA 200.7]

# ICP-MS detection of toxic trace elements

Worldwide regulations require the analysis of toxic trace elements, including As, Cd, Hg, and Pb. ICP-MS accurately measures regulated elements from ppm down to ppt levels.

You can achieve faster ICP-MS analysis—less than 60 seconds per triplicate measurement using the Agilent Integrated Sample Introduction System (ISIS 3).

Here, the ESI prepFAST sampler was coupled to the Agilent 7900 ICP-MS to accurately measure all regulated elements in NIST SRM 1643f (diluted 1/10), according to US EPA Method 200.8.

Element/Mode	Expected Value (ppb)	Average Found (ppb)	Recovery (%)
7 Li [no gas]	17.4	17.5	101
9 Be [no gas]	14.0	14.0	100
11 B [no gas]	157.9	170.0	108
23 Na [He]	20740.0	19652.7	95
24 Mg [He]	8037.0	7553.2	94
27 Al [He]	141.8	140.5	99
39 K [He]	2034.0	1929.0	95
44 K [He]	32300.0	29053.3	90
51 V [He]	37.9	35.0	92
52 Cr [He]	20.4	18.4	90
55 Mn [He]	39.0	37.1	95
56 Fe [He]	98.1	96.1	98
59 Co [He]	27.1	26.1	96
60 Ni [He]	62.4	60.9	98
63 Cu [He]	22.8	21.9	96
66 Zn [He]	78.5	77.0	98
75 As [He]	60.5	57.1	94
78 Se [He]	12.0	11.7	98
88 Sr [He]	323.1	307.5	95
95 Mo [He]	121.4	108.9	90
107 Ag [He]	1.1	0.9	83
111 Cd [He]	6.6	5.7	87
121 Sb [He]	58.3	55.4	95
137 Ba [He]	544.2	490.1	90
202 Hg [He]	NA	<dl< td=""><td>NA</td></dl<>	NA
205 TI [He]	7.4	6.8	91
208 Pb [He]	19.6	17.9	91
238 U [He]	NA	<dl< td=""><td>NA</td></dl<>	NA



# Worried about the time, complexity, and cost of migrating your methods to ICP-MS?

The Agilent 7800 ICP-MS Water Analyzer provides a complete workflow solution. Based on the proven Agilent 7800 ICP-MS system, it enables you to achieve reliable results immediately after installation with:

- High Matrix Introduction (HMI) technology to handle varied, high-matrix samples.
- An optimized method that incorporates the requirements of US EPA 200.8 or ISO 17294-2:2016.
- A Standard Operating Procedure (SOP) and guide.
- A simplified interface that allows any user to achieve reliable results.

### **Emerging contaminants, advanced applications**

Nanoparticles (NPs) are widely used in industrial processes, consumer products, food additives, healthcare, agriculture, and drug delivery. The limited understanding about NP fate and environmental impact is of particular concern. Agilent ICP-MS systems use a single-particle analysis software module to accurately characterize NPs in environmental samples.

The following example demonstrates the different types and numbers of NPs found in an indoor, outdoor, and a children's pool.

	TiO <sub>2</sub> (ng/L)	ZnO (ng/L)
Deionized water	Not detected	Not detected
Indoor pool	49	Not detected
Outdoor pool 1	309	146
Outdoor pool 2	427	1040
Outdoor pool (children's pool)	1100	1610

Concentration of  $TiO_2$  and ZnO NPs in swimming pool water samples. [5994-0310EN: Measuring Multiple Elements in Nanoparticles Using spICP-MS]

# 

Indoor pool

Outdoor pool 3 (children's pool)



Time resolved data for ZnO NPs in three swimming pool water samples



The **Cary 60 UV-Vis** with fiber optic dip probe coupler enables direct measurement in any sample container, eliminating the need for cuvettes and sample transfers.

# UV-Vis determination of concentration levels for nitrates, phosphates, fluorides, and other ions

We ran two tap water samples from different sources (A and B). Both were prepared for analysis and measured using the Agilent Cary 60 UV-Vis equipped with quartz fiber optic dip probe.

Sample	Sample Conc. (mg/L)	Mean Abs	SD	% RSD	Raw Abs
					0.0520
A	0.145	0.0510	0.0009	1.78	0.0504
					0.0506
В	0.709	0.1825			0.1797
			0.0025	1.36	0.1838
					0.1841

Raw data and statistics for nitrate determination in two water samples using UV-Vis. [5990-7932EN: Nitrate Analysis of Water Using the Quartz Fiber Optic Dip Probe on the Cary UV-Vis]

# Sample Preparation, Columns, and Supplies

Reliable, accurate results with fewer repeated samples



Agilent brings you innovative sample preparation products, columns, and supplies for your water testing needs. All are engineered or selected by experienced design teams, manufactured to demanding specifications, and tested under strict conditions.

### Agilent Bond Elut sample prep products: your first choice for solid phase extraction (SPE) analysis

Ensure accurate, reproducible results right from the start. Agilent Bond Elut sample preparation products allow you to efficiently and quantitatively extract the analytes you're looking for from any water sample. You get the benefits of:

- **Faster flow rates.** Uniform particles with a narrow size distribution ensure optimal flow characteristics for sample addition and elution during SPE.
- **Excellent cartridge-to-cartridge reproducibility.** Bond Elut sorbent particles are manufactured using proprietary polymerization techniques to eliminate fines and achieve a narrow particle size distribution.
- Less wasted time and sample. The absence of media fines significantly reduces cartridge clogging. This is critical in high-throughput environments, where SPE must be performed unattended and overnight.
- More reliable data. A proprietary QC process confirms the correct particle size while delivering superior flowthrough.
- Greater stability. Bond Elut trifunctional bonding chemistry is more hydrophobic than monofunctional bonding.
- A wide range of manifolds and accessories. Choose from flexible configurations available as individual components or complete assemblies.

Bond Elut SPE products support water analysis with over 40 bonded silica phases for high-specificity methods. In addition, polymeric phases for rapid method development increase selectivity with highly specific SPE extractions to improve detection limits and increase method ruggedness.



# Determining haloacetic acids in water by GC/µECD using SPE

Disinfection of water is essential to kill pathogens. However, the disinfection process can produce health hazards—including disinfection by-products, such as haloacetic acids (HAAs).

Liquid-liquid extraction (LLE) can be used for HAA analysis. However, SPE offers advantages like increased selectivity, less solvent use, reduced preparation time, and lower costs.

Here, we analyzed two drinking water samples for HAAs. Extraction and concentration were performed with Agilent Bond Elut SAX SPE sorbent. A dual-column Agilent 7890 GC/µECD approach, using Agilent J&W DB-35ms Ultra Inert (UI) and DB-XLB columns, provided consistent, sensitive analysis for the derivatized HAAs.

In the following chromatograms, levels were detectable below the US EPA maximum contaminant levels for HAAs in water. Detection limits for most of the HAAs were 0.05 to 0.5 ng/mL. Analyte recoveries at three fortification levels (0.2 to 2, 1 to 10, and 4 to 40 ng/mL) ranged from 82.5 to 116.5% with RSDs < 3.5%.

#### The SPE technique used in this analysis.



#### Extracted and derivatized drinking water samples



GC/µECD chromatograms for two water samples prepared according to method and analyzed using Agilent J&W DB-35ms UI (p/n 122-3832UI) and DB-XLB (p/n 122-1236) GTC columns. The tap water analysis showed the presence of HAAs, while bottled spring water did not. [5990-8765EN: Determination of Haloacetic Acids in Water by GC/µECD Using Agilent J&W DB-35ms Ultra Inert and DB-XLB Columns]

### Inert flow path

#### Perform trace-level analysis with utmost confidence

By minimizing flow path activity through proprietary chemistries, Agilent Inert flow path solutions ensure accurate quantification and high sensitivity for trace-level analysis.

- Ultra Inert liners, with or without deactivated glass wool, are certified to provide low surface activity and highly reproducible sample vaporization—facilitating delivery of active analytes.
- Inert inlet weldments are treated to prevent adsorption and degradation.
- Ultra Inert gold-plated inlet seals are manufactured using metal injection molding, gold plating, and application of our Ultra Inert chemistry. So you get a leak-free seal that reduces active analyte adsorption.
- Inert MS source ensures sensitivity when analytes reach the mass spectrometer.
- Capillary flow technology purged union lets you backflush high boilers in heavy-matrix samples, increasing column lifetime and system productivity.
- UltiMetal Plus Flexible Metal ferrules are the only ferrules that won't introduce active sites into the flow path.
- Agilent J&W DB-624 UI is the global reference standard for VOC analysis in water and is often the column of choice. The 0.18 mm version provides a fast and comprehensive VOC analysis in less than 15 minutes.
- Gas Clean purifier removes oxygen, moisture, hydrocarbons, and other contaminants.
- Gas Clean filters remove contaminants, ensuring that the highestquality gas flows through the system. So you can maintain flow path inertness and column integrity. Sensors monitor chemical indicators, alerting you when a filter needs replacing.

#### Agilent Inert flow path





Peak identification: 1. 2,4-Dinitrophenol 2. 4-Nitrophenol 3. 4,6-Dinitro-2-methylphenol 4. 4-Aminobiphenyl

5. Pentachlorophenol IS1. Acenaphthene-d10 IS2. Phenanthrene-d10

The **Agilent Inert flow path** provides high responses for sensitive acidic compounds such as semivolatile 2,4 DNP. A standard flow path, similarly configured, shows activity and adsorption. [5990-8532EN: *Lower Your Detection Limits and Quantify Active Analytes* with Confidence, Agilent Ultra Inert Solutions]

# Agilent Inert flow path solutions deliver industry-leading results

Flow path inertness is more than just vital to your analysis; it's also on the cutting edge of GC. Agilent is leading the way with Ultra Inert inlet liners, Ultra Inert columns, and instruments that, together, create the most inert flow path. So you get maximum confidence in your results. To learn more, visit **www.agilent.com/chem/inertflowpath** 



# Proof that GC column inertness can help ensure accurate trace-level detection of pesticides and herbicides in water

Potentially dangerous pesticide residue can enter our water supplies through runoff, or by leaching through soil into groundwater. The EU and US EPA have established regulations for maximum pesticide levels in drinking water.

Column and liner inertness are critical to achieving consistently reliable measurements, especially for pesticides such as endrin and DDT. These pesticides are particularly susceptible to interactions with active sites in the inlet or on the column.

This application example uses an Agilent J&W Ultra Inert column and liner to help create an inert sample flow path. Thirty-seven targeted chlorinated pesticides and herbicides were resolved on the Agilent J&W DB-35ms Ultra Inert primary analysis column and the Agilent J&W DB-XLB confirmation column—and it took less than 23 minutes.



#### GC columns with Smart Key: Compliment your inert flow path

Smart Keys identify and monitor your GC column. They reduce manual input errors for method parameters and optimize maintenance schedules.





Enlarged GC/µECD chromatogram section of a 10 ng/mL chlorinated pesticide standard. The analysis was performed on an Agilent J&W DB-35ms Ultra Inert 30 m x 0.32 mm, 0.25 µm column. Note the excellent peak response and resolution. [5990-9735EN: Sub µg/L Level Analysis of Chlorinated Pesticides and Herbicides in Water by GC/µECD Using Agilent J&W DB-35ms Ultra Inert and DB-XLB Columns]

# Agilent Reference Materials

More than 5,000 chemical reference standards, all in one place

No matter what type of application workflow you are running, the success of your analysis depends on your initial calibration. That means you need to be sure that your standards are of the highest quality. Agilent standards are rigorously tested and contaminant free, so you can calibrate with confidence—and maximize accuracy.

## Complete your water workflow solution

Here's a small sampling of the Agilent Certified Reference Materials (CRMs) and Reference Materials (RMs) portfolio. All come with Certificates of Analysis and Safety Data Sheets.

- US EPA Method 500 Series: drinking water standards
- US EPA Method 600 Series: wastewater standards
- US EPA Method 8000 Series: groundwater standards
- US EPA Method 200.7: multielement standards for metals in water and wastes by ICP-OES
- US EPA Method 200.8: multielement standards for trace metals in water and wastes by ICP-MS
- US EPA Method 6010C: multielement standards for trace elements in groundwater, soil, sediment, and solid waste by ICP-OES
- Certified Lab (CLP) Standards
- Individual and mixes of:
  - Pesticides
  - PAHs
  - Volatiles and semivolatiles
  - Dioxins and furans
  - PCBs and PBBs
  - Halocarbons
  - Petrochemicals
- Inorganic analytes:
  - Single element
  - Multielement
  - Custom





If you cannot find the standards you are looking for, or to see the full catalog, go to **www.agilent.com/ chem/standards**. You can also order quality custom organic and inorganic standards from our website.

# InfinityLab Poroshell 120 Columns

Fast, rugged, high-resolution separations





# The InfinityLab Poroshell 120 family has grown to include 18 chemistries—including new phases for chiral and HILIC separations. Their benefits include:

- **Analytical efficiency.** The porous outer layer and solid core limit diffusion distance and improve separation speed, while narrow particle size distributions improve resolution.
- Up to 18 chemistries. This wide range of innovative chemistries supports optimal separation of diverse analytes and enables fast method development.
- Excellent lot-to-lot reproducibility. A proprietary, single-step porous shell process dramatically reduces tiny differences between lots and columns.
- A scalable family of particles. 1.9 μm, 2.7 μm, and 4 μm superficially porous particles enable you to get the best from all your methods and instruments.
- Long column life. Robust Poroshell particles and chemistries are stable at required pressures.
  UHPLC guard columns further extend the life of your analytical column.
- Column ID. Get the information you need for the highest-quality results on your InfinityLab Series LC. Preprogrammed ID tags allow you to track column properties and use parameters. These include column identity, lot and batch number, last injection date, number of injections, and maximum temperature used.

### Easily transfer methods for fast, accurate results in environmental analyses

Poroshell 120 phases use ZORBAX bonding processes. So you can be sure of easy scalability and method transfer.

In this example, we replaced a ZORBAX Eclipse Plus C18 column (4.6 x 100 mm, 5  $\mu$ m) with an InfinityLab Poroshell 120 EC-C18 column. This change significantly cut analysis times for environmental phenols in water, while delivering equivalent peak capacity and resolution.



Method scalability between Agilent ZORBAX Eclipse Plus C18 and Agilent InfinityLab Poroshell 120 EC-C18 columns

Separating nine phenol compounds at 182 bar. In just six minutes, an Agilent InfinityLab Poroshell 120 EC-C18, 4.6 x 50 mm column (bottom) provided the same peak capacity as the original method (top). [5990-6156EN: Fast Analysis of Environmental Phenols with Agilent Poroshell 120 EC-C18 Columns]

# The "small" parts of your workflow make a big difference in the quality of your results

Agilent InfinityLab supplies are designed and manufactured to optimize your LC and MSD workflows, making your everyday tasks more efficient.



# Informatics Software

Powerful support for your water safety efforts



### **Agilent MassHunter software**

#### Find the answers you seek

The advanced data mining and processing tools in our MassHunter suite help you quickly and accurately extract available information from the analytes in your samples.

- Enable powerful data collection, processing, and reporting tools. So you can breeze through application-specific workflows with comprehensive support of GC and GC/MS technology.
- **Use one software** for all Agilent GC and GC/MSD instruments, including single quadrupole, tandem quadrupole, and Q-TOF.
- **Analyze complex environmental samples** with compound-based analysis and reporting workflows using MassHunter Quantitative Analysis with Quant-My-Way customization.
- **Simplify data analysis** with powerful application-specific software, such as personal compounds, databases, and libraries.



### Agilent CrossLab: real insight, real outcomes

CrossLab goes beyond instrumentation to bring you services, consumables, and lab-wide resource management. So your lab can improve efficiency, optimize operations, increase instrument uptime, develop user skill, and more. Agilent CrOSSLab From Insight to Outcome

Learn more:

www.agilent.com/chem/environmental

Buy online: www.agilent.com/chem/store

Find a local Agilent customer center in your country: www.agilent.com/chem/contactus

USA and Canada: 1-800-227-9770 agilent\_inquiries@agilent.com

Europe info\_agilent@agilent.com

Asia Pacific inquiry\_lsca@agilent.com

Agilent Trusted Answers

This information is subject to change without notice.

© Agilent Technologies, Inc. 2019 Published in the USA, May 7, 2019 5991-0350EN