

Water Quality Applications

THE MEASURE OF PURITY

The Measure of Confidence



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Safeguarding a Precious Resource

Like you, Agilent is committed to ensuring the quality of our water supply

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 recognized every year.

From large cities to remote villages, the infrastructure needed to make water safe for human consumption – and transport it to where it's needed – is either aging or nonexistent. To ensure the safety of this essential resource, and to protect human health, governments and private institutions are continuously monitoring and regulating the quality of our water. Agilent is helping to ensure the success of this effort by providing high-productivity, high-throughput tools to efficiently and reliably monitor water quality. With optimized solutions for organic and inorganic detection, the most sensitive detectors on the market, and strategies for minimizing matrix interference, Agilent helps you achieve the selectivity and low limits of detection (LOD) you need to confidently measure the chemical contaminants that threaten the global water supply.



Agilent's 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 by combining an expanded portfolio of analytical products with unrivaled leadership in water quality measurement.

As water analysis needs change, we will continue to offer the most accurate, sensitive, and reliable solutions that ensure confidence in the quality of this valuable resource.



Volatiles

By adding new features to minimize cycle times and increase throughput, Agilent has enhanced the performance of our volatiles measurement products – boosting your productivity while retaining Agilent's hallmark sensitivity and reliability.

Semi Volatiles and Pesticides

Our sensitive instruments for semi volatiles and pesticides measurement overcome the challenges of matrix interference, resulting in high-resolution measurements with low LOD. New Online SPE LC/MS/MS solutions can reduce sample prep time, while decreasing manual labor.

Emerging Contaminants

Agilent's portfolio of LC/MS, GC/MS and ICP-MS products combine high sensitivity with rapid, reliable analysis of emerging contaminants for greater productivity.

Inorganic and Elemental

Enhancements to our inorganic product line have created a comprehensive portfolio for demanding measurements over a wide dynamic range – from parts-per-trillion to parts-per-hundred.

Sample Preparation, Columns and Supplies

Your best results start with Agilent sample preparation products for selective interference removal, and Agilentengineered columns and supplies for speed, resolution, and sensitivity.

Informatics Software and Services

Unmatched expertise, informatics, and services support your water safety efforts.



Volatiles Measurement Greater productivity, sensitivity, and reliability

Volatile organic compounds (VOCs) enter our water supply in a number of ways. Industrial processes, biological contamination and water disinfection treatments all produce VOCs that can increase the risk of cancer, damage organs, and cause disease. In order to reduce the risks associated with these compounds, many governments closely regulate the amounts that are allowed in drinking water.

Agilent provides the tools you need to monitor trace volatile materials in the environment. Our full range of automated sampling devices and traps lets you choose the most effective sampling method for your application – whether you need the simplicity and speed of static headspace sampling, the sensitivity of purge and trap sampling, or the convenience of solid phase micro-extraction (SPME) sampling.

By combining robust instruments and columns with the latest features for minimizing cycle times and maximizing throughput, Agilent equips you for high-productivity measurement of VOCs in water – from regulated pollutants to hydrocarbons.



Agilent's 5977A Series GC/MSD with 7697A Headspace Sampler. Headspace sampling ensures an inert sample pathway for for superior GC/MSD performance without analyte degradation or loss.



Flexible solutions for sample introduction and detection High-capacity headspace sampling

Agilent's 7697A Headspace Sampler provides high sample capacity and built-in Electronic Pneumatic Control (EPC) to ensure superior performance over a wide concentration range. Its inert sample pathway prevents analyte degradation or loss, with sensitivities lower than U.S. EPA and EU directives.

Analysis by headspace extraction is a direct approach for volatiles in water, because it transfers less water to the GC, has few parameters to adjust and is easy to implement. During headspace sampling, vials containing samples 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 aloquot is delivered to the GC via a loop.

When used with Selected Ion Monitoring (SIM), headspace sampling can also achieve part-per-trillion levels of detection.

GC/MS analysis of tap water using the Agilent 7696A Headspace Sampler, followed by separation and detection with Agilent's 7890B GC/5977A Series GC/MSD system

In this example, the 5977A GC/MSD was operated in simultaneous SIM/SCAN mode with the trace ion detection mode switched on. The MSD was also equipped with the triple axis detector (TAD) and an extractor lens.

This application meets European Union requirements for volatiles in water as outlined in 98/83/EC Directive. Calibration from 0.05-20 ppb showed excellent % 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	? <mark>×</mark>
Options	
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
⊡- External Standard Compounds	*
Dichlorodifluoromethane	=
Chloromethane	-
Vinyl Chloride	
Bromomethane	
Chloroethane	
Trichlorofluoromethane	
- 1,1-Dichloroethene	
Dichloromethane	
- 1,2-Dichloroethene (trans)	
- 1,1-Dichloroethane	
- 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 succ	cessful.

Agilent MassHunter 5977 data analysis - existing MSD Chemstation data analysis methods are easily converted to MassHunter methods.



Agilent MassHunter Data Analysis Software - Vinyl Chloride calibration from 0.10-40 ppb. [5991-2108EN Environmental VOCs using Agilent Headspace sampler with 7890B GC/5977A GC/MSD]

Sensitive purge and trap autosampling

Agilent distributes the following purge and trap instruments, which combine high-sensitivity VOC detection with low carryover – giving you ultimate confidence from sample to sample.

- Teledyne Tekmar Stratum Purge and Trap Concentrator (PTC)

 a sample preparation instrument that removes Volatile
 Organic Compounds (VOCs) from aqueous and solid samples using Helium or Nitrogen.
- Teledyne Tekmar AQUATek 100 Autosampler a Purge and Trap (P&T) autosampler that automates the sample preparation steps for P&T analysis of liquid samples. Ideal for samples such as drinking water and wastewater.
- Teledyne Tekmar Atomx Automated VOC Sample Prep System – combines an autosampler and P&T into a single instrument for analyzing VOCs in soils and waters. This is the first and only system that employs a unique methanol extraction automation feature for high-level soils in accordance with U.S. EPA Method 5035.

Optimized VOC analysis in drinking water using Purge and Trap

The chromatogram on page 7 represents the analysis of volatiles in drinking water according to US EPA Method 524.2. The analytical system is the Teledyne Tekmar Atomx sample prep system interface to an Agilent 7890/5975C GC/MSD system.

An Agilent VOC applications kit (p/n G7022A) was used to provide optimum method parameters and instrument conditions to ensure the best sensitivity, robustness, and stability while meeting all the required QA/QC of this EPA method.

A calibration curve ranged from 0.25-50 μ g/L routinely produced VOC average response factors less than 20% relative standard deviation (RSD).





Total Ion Chromatogram (TIC) of Method 524.2 Initial Calibration standard. Inset: Extracted Ion Chromatogram of the gases. [5991-0896EN Optimized Volatile Organic Compound Analysis using Purge and Trap with the 5975C GC/MS]

VOC TekLink software allows you to enter all analysis parameters; once activated, it continuously monitors the system to make sure operating limits are not exceeded. The software can also perform useful diagnostics, such as leak and benchmark tests for instrument validation. All instrument parameters, method scheduling and editing can be programmed.

In addition, pre-developed methods are provided for easy startup with little or no modifications. An optional 21 CFR Part 11 data audit trail package is also available.

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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.

Zone section monitors actual values compared to method-driven set points.



Semi Volatiles and Pesticides Measurement

High performance with rugged dependability

Semi volatile organic compounds and pesticides can remain in the environment for a long time, presenting a constant threat to our water supply. Like volatile organic compounds, semi volatiles and pesticides may cause long-term health effects, and are regulated pollutants. However, they can be tough to accurately quantify – especially when present in low concentrations.

GC/MS solutions for pesticides Maintaining sensitivity and inertness in the face of matrix interference

Agilent's mass spectrometers are known for their robustness, as well as their sensitivity in the ppb and ppt range. In addition, Agilent gives you the advantage of these leadingedge technologies designed to eliminate matrix interference:

- Deconvolution reporting software (DRS) reduces the impact of matrix interference through robust algorithms that deconvolute overlapping spectra, increasing the sensitivity of semi volatile and pesticide detection.
- **Retention time locking (RTL) software** reproduces retention times within hundredths of a minute from one Agilent GC system to another. The benefits are twofold: increased throughput and greater confidence in your results.



- Agilent's 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 consistently high performance. Backflushing can significantly improve analytical results and increase sample throughput.
- Flexible comprehensive MRM database reduces the time to create GC/QQQ pesticide methods. Contains MRM transitions and retention times for over 1,000 pesticides and pollutants.
- **Analyzer solutions** are pre-configured and chemically tested, helping you accurately confirm target analytes in complex matrices.



Together, Agilent's 5977A Series 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.



Triple quadrupole mass spectrometry drastically reduces or eliminates interferences that may reduce accuracy and negatively affect detection limits in traditional GC/MS SIM methods.

Agilent 7000 Series Triple Quadrupole GC/MS Perform sensitive, multiresidue analyses in complex matrices

High-boiling molecules that flood out of the GC column at the end of the separation create special challenges for the ion source and mass analyzer. For complex matrices typically separated by GC/MS/MS, this concentration of high boilers can be a worst-case scenario.

Agilent's 7000B 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 this high temperature, and at vacuum, it stays clean even with

complex, high-boiling samples. This eliminates frequent, time-consuming maintenance and improves mass analyzer performance.

In the example here, eight polycyclic aromatic hydrocarbons (PAHs) and six Polybrominated Diphenyl Ethers (PBDEs) were extracted from wastewater with no clean-up, and analyzed on the Agilent 7000 Series Triple Quadrupole GC/MS. The desired detection was achieved with 25 μ L injections using the Agilent MMI in solvent vent mode. Labeled analogues were used as internal standards for each compound of interest.



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



This screen capture of Agilent's 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 0-10 ppt.

This list shows eight polycyclic aromatic hydrocarbons identified by the EPA as possible human carcinogens; it also shows six PBDE compounds 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 µg/L)

naphthalene (2.0)beanthracene (0.1)pofluoranthene (0.1)pobenzo(b)fluoranthene (0.015)pobenzo(k)fluoranthene (0.015)pobenzo(a)pyrene (0.05)poindeno(123cd)pyrene (0.001)po

benzo(ghi)perylene (0.001) polybrominated diphenyl ether (PBDE) 28 polybrominated diphenyl ether (PBDE) 47 polybrominated diphenyl ether (PBDE) 99 polybrominated diphenyl ether (PBDE) 100 polybrominated diphenyl ether (PBDE) 153 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 clean-up, 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 solutions for pesticides Quantify trace-level herbicides in drinking water with the Agilent 1200 Infinity Series Online SPE Solution

Whether you need to enrich your analytes, remove matrix components, or lower detection limits for trace-level water analysis, the modular design of the Agilent 1200 Infinity Series Online SPE Solution provides you with the flexibility to tailor your system to match virtually any analytical challenge.

Agilent's Online SPE Solution is based on the 1290 Infinity Flexible Cube coupled with a 6400 Series Triple Quadrupole Mass Spectrometer. The flexible cube houses re-usable SPE cartridges and up to two valves. Valve heads are easy to mount on the valve drives thanks to Agilent's Quick-Change valve technology. A built-in pump flushes the sample onto the cartridges.

An extensive portfolio of valves makes it easy to customize your Online SPE system to fit your needs. Combine these kits with the SPE starter set for applications such as:

- Direct injection
- Multi-SPE

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Acquisition time (min)

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- · High volume injection, or
- Flask sampling

The high precision and accuracy of the Agilent 1200 Infinity Series Online SPE Solution could be demonstrated in the analysis of herbicides at trace levels down to 1 ppt (LOQ) in drinking water.

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 1200 Infinity Series Online SPE Solution

MRM chromatograms for a calibration standard with a concentration of 100 ppt (ng/L) each for herbicides measured by an Online SPE LC dynamic MRM method with quantifier and qualifier ions.

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Agilent's Pesticide Triggered MRM (tMRM) LC/MS Application Kit is truly unique, because much of the development work has already been completed. The kit features easy-to-use examples that demonstrate how to set up screening methods and quickly adapt them to your specific needs. It also includes:

- A tMRM database and library for more than 700 pesticides that includes compound names, up to 10 MRM transitions, fragmentor voltages, collision energies, and the ability to add retention times for each database compound for reliable pesticide screening with tMRM library verification.
- **Pretested analysis methods**, using the tMRM database, are provided for target screening of pesticides that are routinely monitored around the world.



Total ion MRM chromatogram of 0.5 µg/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

Over the past decade, pharmaceutical and personal care products (PPCPs), perfluorinated organics (PFCs) and endocrine disruptors have been identified as new chemical threats to our water supply. 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 – with LC/MS and GC/MS systems that provide sensitive detection and identification of a wide range of trace analytes.

Trace-level detection of polar compounds: analyze hundreds of analytes per injection

The high polarity and extremely low levels of many PPCP and PFC contaminants make LC/MS analysis the method of choice. Agilent's 1290 Infinity LC, coupled with Agilent's 6400 Series Triple Quadrupole LC/MS provides fast, multi-analyte quantitation with multiple reaction monitoring (MRM) at rates of 200 per second or faster.





Agilent's 6400 Series Triple Quadrupole LC/MS and 1290 Infinity LC meet your needs for target compound analysis.

Sensitive and accurate detection of PPCPs in water

For targeted screening of known PPCPs and PFCs, the unmatched sensitivity and extremely fast MRM switching speeds make Agilent's 6400 Series Triple Quadrupole systems ideal tools for analysis.



Confirming the presence of two PPCPs in surface water by direct aqueous injection into Agilent's 6400 Series LC/MS. The qualifying ion abundances for these two 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.]

Analysis of drinking water

Here, a group of perfluorinated carboxylates (PFCAs) and sulfonates (PFSAs) were screened at low-level fg on-column in a potable water matrix with zero background interference using dynamic MRM. This approach allowed us to gain reliable, positive identifications and extremely low limits of detection.

Compounds	LOD (fg on-column, S/N >3)
perfluoro-1-butanesulfonate (PFBS)	5
perfluoro-n-hexanoic acid (PFHxA)	8.4
perfluoro-n-heptanoic acid (PFHpA)	12.2
perfluoro-1-hexanesulfonate (PFHxS)	2.6
perfluoro-n-octanoic acid (PFOA)	43.7
perfluoro-n-nonanoic acid (PFNA)	75
perfluoro-1-octanesulfonate (PFOS)	5.7
perfluoro-n-decanoic acid (PFDA)	36.3
perfluoro-n-undecanoic acid (PFUA)	44
perfluoro-1-decanesulfonate (PFDS)	3.2
perfluoro-n-dodecanoic acid (PFDoA)	55.9
perfluoro-n-tridecanoic acid (PFTriA)	74.2
perfluoro-n-tetradecanoic acid (PFTA)	21.7

LOD results for drinking water samples. [5990-5313EN A Low Femtogram Target Screen Method for Perfluorinated Compounds in Food Matrices and Potable Water Using the Agilent 6460 Triple Quadrupole LC/MS System Equipped with Agilent Jet Stream Technology.]



PFC suite dynamic MRM chromatogram (overlaid) at 100 fg with quantifier and qualifier ions. [5990-5313EN A Low Femtogram Target Screen Method for Perfluorinated Compounds in Food Matrices and Potable Water Using the Agilent 6460 Triple Quadrupole LC/MS System Equipped with Agilent Jet Stream Technology.]

Unambiguous structural determination of unknowns

With their sub-ppm mass accuracy and ultra high definition, Agilent's GC and LC Accurate-Mass Q-TOFs can help you reduce uncertainty, minimize false positives, improve database search scores, and generate molecular formulas for unknowns. Their enhanced resolving power of up to **40,000** reliably detects mass peaks of interest, while a dynamic range of up to five orders in-spectrum uncovers lowabundance compounds in the presence of higher-abundance components.



Agilent 1290 Infinity LC and 6500 Series Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) LC/MS



Extracted ion chromatogram of phenazone at the 10 ng/L level, with the structure of the compound (inset).



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



Inorganic and Elemental Analysis Detecting 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. But no matter what the cause, monitoring the levels of these contaminants in drinking, natural, and environmental waters is essential for ensuring water quality and protecting human health.

One of the biggest challenges is monitoring multiple metals in a large number of samples, where quantities may range from trace levels to high concentrations. Agilent's portfolio of high-productivity instruments delivers sensitive, accurate, and precise measurements across a wide dynamic range – from percentage down to low ppt, and in the presence of matrix interference.

Each instrument has unique performance characteristics, allowing you to choose the technique that meets your analytical needs (detection limits, measurement range, and elemental coverage), as well as your demands for sample matrix levels, 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%								
1-1000 ppm								
100-1000 ppb								
1-100 ppb								
ppt								
	N	umber of S	Samples					
Few								
Several								
Many								
	Number	of Elemen	its per Sam	ple				
Single								
Few (2-5)								
Intermediate (5-10)				•	•			
Many								
Sample Matrix								
< 3% solids								
3-10%								
> 10%								



Detecting trace metals in water using atomic absorption

Agilent's dedicated 280Z Zeeman Graphite Furnace AAs deliver greater sensitivity with extended tube lifetimes – making GFAA a suitable alternative for analyzing heavy metals on a limited budget, or as a back-up to ICP-0ES.

Mercury is one of the most toxic heavy metals in the environment and is routinely monitored in water. U.S. EPA method 245.1 for determining mercury in industrial effluents and drinking, surface, ground, sea, and brackish waters

Element	MDL (µg∕L)	Element	MDL (µg/L)
As	0.5	Ni	0.6
Be	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	ТІ	0.7

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

relies on the proven cold vapor AA technique with stannous chloride as the reducing agent. Combining Agilent's VGA 77 Vapor Generation Accessory with the AA240 Series offers a number of advantages for this approved method.

· High sample throughput and full automation capabilities.

• **Precise, accurate results** with a Hg detection limit of 0.05 μ g/L. Precision is typically better than 1% at the 2-3 μ g/L level with 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 7700 Series ICP-MS provides unparalleled accuracy in high-matrix samples, redefining cell performance in helium mode with a revolutionary 3rd generation cell design – the ORS³.



Agilent 700 Series ICP-OES Spectrometers feature axial plasma viewing and simultaneous wavelength measurement for extended dynamic range and reduced interference.



Agilent 4100 Microwave MP-AES performs multi-element determination in water using a plasma that runs on air for lowest cost of ownership.



Agilent 240AA Series AAS is built for very low detection limits (low ppb or ppt).

High-volume, high productivity analysis of trace metals in water

ICP-OES is a commonly used analytical technique for water analysis around the world. Agilent's Inductively Coupled Plasma Optical Emission Spectrometers (ICP-OES) offer the finest performance, productivity and flexibility, making them ideal for determining trace and toxic elements in waters. To test the capabilities of the 700 Series ICP-OES, we determined 22 analytes in a certified reference water sample *(NIST 1643e Trace Elements in Water).* The tables below confirm excellent agreement with the certified results as shown by % recovery. In addition, the measured contract required detection limits (CRDLs) easily exceed the specified CRDLs.

Results for determining 22 analytes in a certified reference water sample (NIST SRM 1643e Trace Elements in Water)

Note the excellent agreement with certified values for all analytes, demonstrating the accuracy possible with the Agilent 700 Series ICP-OES.

Element	NIST 1643e Certified (mg/L)	NIST 1643e Measured LCS (mg/L)	LCS % Recovery	Element	NIST 1643e Certified (mg/L)	NIST 1643e Measured LCS (mg/L)	LCS % Recovery
Ag 328.068	0.001062	<crql< td=""><td>-</td><td>K 769.897</td><td>2.034</td><td>2.11</td><td>103.7</td></crql<>	-	K 769.897	2.034	2.11	103.7
AI 237.312	0.1418	0.151	106.6	Mg 285.213	8.037	8.55	106.4
As 188.980	0.06045	0.0590	97.5	Mn 257.610	0.03897	0.0410	105.1
Ba 585.367	0.5442	0.554	101.9	Na 589.592	20.74	21.6	104.1
Be 313.042	0.01398	0.0140	100.0	Ni 231.604	0.06241	0.0629	100.9
Ca 315.887	32.3	32.0	99.0	Pb 220.353	0.01963	0.0207	105.7
Cd 214.439	0.006568	0.00642	97.8	Sb 217.582	0.0583	0.0602	103.2
Co 228.615	0.02706	0.0280	103.5	Se 196.026	0.01197	<crql< td=""><td>-</td></crql<>	-
Cr 267.716	0.0204	0.0209	102.4	TI 190.794	0.007445	<crql< td=""><td>-</td></crql<>	-
Cu 324.754	0.02276	0.0229	100.7	V 292.401	0.03786	0.0389	102.7
Fe 238.204	0.0981	0.105	106.8	Zn 206.200	0.0785	0.0803	102.3

Laboratory Control Sample (LCS): NIST SRM 1643e trace elements in water. [5990-7918EN Ultra-fast ICP-OES Determination of Trace Elements in Water, Conforming to U.S. EPA 200.7 and Using Next Generation Sample Introduction Technology.]

Element	Sample Measured (mg/L)	Sample + Spike Measured (mg/L)	Added Spike Conc. (mg/L)	Spike % Recovery	Element	Sample Measured (mg/L)	Sample + Spike Measured (mg/L)	Added Spike Conc. (mg/L)	Spike % Recovery
Ag 328.068	<crql< td=""><td>0.0484</td><td>0.0491</td><td>98.6</td><td>K 769.897</td><td>0.597</td><td>-</td><td>-</td><td>-</td></crql<>	0.0484	0.0491	98.6	K 769.897	0.597	-	-	-
AI 237.312	0.0939	2.11	1.96	103	Mg 285.213	1.114	-	-	-
As 188.980	<crql< td=""><td>0.0395</td><td>0.0361</td><td>109</td><td>Mn 257.610</td><td>0.00614</td><td>0.524</td><td>0.491</td><td>105</td></crql<>	0.0395	0.0361	109	Mn 257.610	0.00614	0.524	0.491	105
Ba 585.367	0.0176	2.05	1.96	104	Na 589.592	4.074	-	-	-
Be 313.042	<crql< td=""><td>0.0513</td><td>0.0491</td><td>104</td><td>Ni 231.604</td><td><crql< td=""><td>0.516</td><td>0.491</td><td>105</td></crql<></td></crql<>	0.0513	0.0491	104	Ni 231.604	<crql< td=""><td>0.516</td><td>0.491</td><td>105</td></crql<>	0.516	0.491	105
Ca 315.887	3.64	-	-	-	Pb 220.353	<crql< td=""><td>0.0201</td><td>0.018</td><td>112</td></crql<>	0.0201	0.018	112
Cd 214.439	<crql< td=""><td>0.0486</td><td>0.0451</td><td>108</td><td>Sb 217.582</td><td><crql< td=""><td>0.101</td><td>0.0901</td><td>112</td></crql<></td></crql<>	0.0486	0.0451	108	Sb 217.582	<crql< td=""><td>0.101</td><td>0.0901</td><td>112</td></crql<>	0.101	0.0901	112
Co 228.615	<crql< td=""><td>0.51</td><td>0.491</td><td>104</td><td>Se 196.026</td><td><crql< td=""><td>0.0493</td><td>0.0451</td><td>109</td></crql<></td></crql<>	0.51	0.491	104	Se 196.026	<crql< td=""><td>0.0493</td><td>0.0451</td><td>109</td></crql<>	0.0493	0.0451	109
Cr 267.716	<crql< td=""><td>0.206</td><td>0.196</td><td>105</td><td>TI 190.794</td><td><crql< td=""><td>0.0474</td><td>0.0451</td><td>105</td></crql<></td></crql<>	0.206	0.196	105	TI 190.794	<crql< td=""><td>0.0474</td><td>0.0451</td><td>105</td></crql<>	0.0474	0.0451	105
Cu 324.754	0.162	0.412	0.246	102	V 292.401	<crql< td=""><td>0.503</td><td>0.491</td><td>102</td></crql<>	0.503	0.491	102
Fe 238.204	0.0924	1.1	0.982	103	Zn 206.200	0.00637	0.53	0.491	107

Results for a certified wastewater sample: High Purity Standards CWW-TM-C analyzed by ICP-OES. [5990-7918EN Ultra-fast ICP-OES Determination of Trace Elements in Water, Conforming to U.S. EPA 200.7 and using Next Generation Sample Introduction Technology.]

ICP-MS analysis of metals in drinking water

Recent drinking water regulations require the low-level analysis of specific chemical forms of elements such as hexavalent chromium. ICP-MS can measure all regulated elements in natural and drinking waters, from major elements at ppm to the lowest trace elements at ng/L (ppt) levels.

Element/	Measured		D (0/)
mode	(ppb)	RSD (%)	Recovery (%)
9 Be [no gas]	14.4	2.0	103.3
11 B [no gas]	156.3	1.6	99.0
23 Na [no gas]	19581	2.7	94.4
24 Mg [no gas]	7376.6	2.9	91.8
27 Al [no gas]	137.5	2.8	97.0
39 K [He]	2043.5	0.9	100.5
44 Ca [He]	34251	2.6	106.0
51 V [He]	36.6	0.7	96.9
52 Cr [He]	19.8	1.0	97.2
53 Cr [He]	19.7	0.7	96.6
55 Mn [He]	38.5	0.6	98.9
56 Fe [He]	100.9	1.2	102.9
57 Fe [He]	100.2	1.4	102.2
59 Co [He]	25.8	0.6	95.5
60 Ni [He]	58.2	0.7	93.4
63 Cu [He]	21.1	0.8	92.8
66 Zn [He]	73.2	0.5	93.3
75 As [He]	59.9	2.2	99.2
78 Se [He]	10.9	2.8	91.2
88 Sr [He]	301.5	4.5	93.3
95 Mo [He]	114.9	0.6	94.7
107 Ag [He]	0.94	1.4	88.1
111 Cd [He]	6.32	1.0	96.2
121 Sb [He]	56.2	0.5	96.3
137 Ba [He]	617.1	1.0	113.4
205 TI [He]	6.00	0.7	99.2
208 Pb [He]	18.9	0.2	96.1

Here you can see the mean values, relative standard deviation and % recoveries of certified values for NIST 1643e (1/10 dilution) in standard reference water by ICP-MS. [5990-4313EN The Agilent 7700x ICP-MS Advantage for Drinking Water Analysis.]

Determining concentration levels of nitrates, phosphates, fluorides, and other ions using UV-Vis

The experimental method from *Standard Methods for the Examination of Water and Wastewater* can be used to determine nitrate levels over a concentration range from 0-7 mg/L by measuring the absorbance at 220 and 275 nm. This allows correction for interferences due to dissolved organic matter. To increase sample throughput and efficiency, optical fibers may be used to measure sample absorbance. This allows for on- or off-site analysis, which is more appealing than a conventional cuvette.

In the analysis below, we ran two tap water samples from different sources (A and B). Both were prepared for analysis and measured using the Agilent Cary UV-Vis equipped with quartz fiber optic dip probe, which proved to be a highly precise, efficient technique for determining the nitrate content in water.

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

This table lists the raw data and statistics for the determination of nitrate 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.]



The Cary UV/VIS with Fiber Optic Dip Probe Coupler delivers unsurpassed photometric accuracy and linearity, superior optical stability, and high spectral resolution.



Sample Preparation, Columns and Supplies Reliable, accurate results with fewer repeated samples

As the world's chromatography leader, Agilent is uniquely positioned to bring you innovative sample prep products, GC and LC columns, and supplies for your water testing needs. All are engineered or selected by our experienced design teams, manufactured to our demanding specifications and tested under strict conditions.

Agilent Bond Elut Sample Prep Products

Your first choice for SPE analysis

Robust, reliable analysis of water samples begins with highquality sample preparation and extraction.

Agilent's Bond Elut sample preparation products allow you to *efficiently and quantitatively* extract the analytes you're looking for from any water sample – including surface water, wastewater, river water, and tap water. So you can ensure accurate, reproducible results right from the start. Bond Elut products deliver:

- 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 very 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 flow-through.
- **Greater stability:** Bond Elut's 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 complement increased instrument selectivity with high-specificity SPE extractions to improve detection limits and increase method ruggedness.



Determining haloacetic acids in water by GC/µECD using solid phase extraction (SPE)

Most people assume chlorinated water is safe to drink. However, the chlorination process itself can produce health hazards – including disinfection byproducts, such as haloacetic acids (HAAs).

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

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

Flow chart for the SPE technique used in this analysis

Add 0.5 mL aq NH₄CL to 50 mL water sample.

Adjust pH of sample to pH5 \pm 0.5 with sulfuric acid as necessary.

Add surrogate, and QC spike solution if necessary.

Assemble glass block manifold and attach SPE cartridges.

Condition Bond Elut SAX SPE cartridges with 10 mL MeOH, followed by 10 mL reagent water.

Add the 50 mL water sample to cartridge while drawing under vacuum at 2 mL/min.

Add 10 mL MeOH to cartridge and draw through at 2 mL/min.

Disassemble vacuum manifold and insert 15 mL screw cap centrifuge tubes.

Add 3 mL 10% H₂SO₄/MeOH to cartridge and elute at 1.5 mL/min.

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. Note that 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 the 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 to produce 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 Ultra Inert GC columns are rigorously tested to ensure exceptionally low bleed and consistently high inertness for optimal active analyte delivery to the GC or MS detector.
- Gas Clean purifier removes oxygen, moisture, hydrocarbons, and other contaminants.

Semi volatiles suitability

Agilent Inert Flow Path



Agilent Inert Flow Path provides high responses for sensitive acidic compounds such as semi volatile 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 liners, Ultra Inert columns, and instruments that, together, create the most inert flow path – giving you maximum confidence in your results.



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

Potentially dangerous pesticide residues can enter our water supplies through runoff, or by leaching through soil into groundwater. Accordingly, the European Union (EU) and United States Environmental Protection Agency (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, which are particularly susceptible to interactions with active sites in the inlet or on the column.

The application example shown below uses an Agilent J&W Ultra Inert column and liner to help create an inert sample flow path. *In less than 23 minutes*, 37 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.



EPA 508.1 low level pesticides peak shape and resolution with an Agilent J&W DB-35ms UI column

Enlarged GC/µECD chromatogram section of a 10 ng/mL chlorinated pesticide standard analyzed 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 Pesticide and Herbicide Analysis In Water by GC/µECD Using Agilent J&W DB-35ms Ultra Inert and DB-XLB Columns.]

Fast LC Columns

Your key to fast, accurate results

When human health and safety are at stake, you cannot afford to let anything jeopardize your productivity and results. That is why Agilent-engineered ZORBAX columns are designed to ensure reproducibility and high efficiency for high-throughput water testing applications.

Optimize your UHPLC with ZORBAX Rapid Resolution High Definition (RRHD) Columns

Agilent ZORBAX Rapid Resolution High Definition (RRHD) columns are the *only* columns stable to 1200 bar, allowing you to push UHPLC instrument and flow rates to the limit and select mobile phases that best suit your separation. Agilent ZORBAX RRHD columns are available in 13 phases, including HILIC.





Here, an Agilent ZORBAX RRHD HILIC Plus column (2.1 mm x 100 mm, 1.8 µm) was used to rapidly analyze Group 4 pharmaceuticals from EPA-1694. [5990-8433EN Fast LC/MS/MS Analysis of Group 4 Pharmaceuticals from EPA-1694 with RRHD HILIC Plus.]

Maximize every HPLC and UHPLC with Poroshell 120 columns

Finally, a Fast LC option that works for *any* HPLC or UHPLC instrument in your lab. Agilent Poroshell 120 columns feature uniquely designed, superficially porous particles that produce high speed and resolution at 40-50% lower backpressures than with sub-2- μ m columns. They are engineered with a 2 μ m frit, which is more forgiving for dirty samples – a common challenge for environmental labs. Because Poroshell 120 phases utilize the same ZORBAX bonding processes, you can be assured of easy scalability and method transfer.

In the example below, we replaced a ZORBAX Eclipse Plus C18 column (4.6 x 100 mm, 5 μ m) with a Poroshell 120 EC-C18 column to significantly cut analysis times for environmental phenols in water, while still delivering equivalent peak capacity and resolution.





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



Informatics Software and Services

Unmatched expertise, informatics, and services support your water safety efforts

Agilent OpenLAB Software

Capture, analyze, and share water quality data

Now it's easy to streamline data management and reporting for all analytical experiments – including organic, inorganic, and emerging contaminant analysis.

OpenLAB ECM (Enterprise Content Management) and OpenLAB ELN (Electronic Lab Notebook) automatically capture and organize data generated during water contaminant analyses. Together, these software solutions enable efficient, reliable water quality monitoring by letting you:

- Plan, execute, and record experiments using customizable templates. You can also configure analytical methods, including those mandated by the EPA.
- Electronically capture and catalog raw data and printed reports from Agilent LC/MS, GC/MS and ICP-MS instruments a consistent, accurate alternative to handwritten notebooks.
- Promote lab-wide collaboration while reducing the time and effort needed to create water quality reports – by simplifying the storage and management of data generated by mass spectrometers.
- Enhance technician productivity by using OpenLAB ECM's central data repository to streamline reporting, review, and signoff.
- Support regulatory compliance with data integrity, traceability, and security.

The **Agilent Professional Services Organization** is a global leader in systems integration consulting, resulting from decades of experience helping some of the world's leading Chemical Analysis companies. Our skilled and dedicated consultants have a profound understanding of business processes coupled with deep industry knowledge.

Delivery teams specialize in the implementation and integration of custom and packaged IT systems, as well as software development that is designed to meet your needs and increase the return on your software investment.



Agilent Services No one works harder to optimize your lab's performance

Every day, chemical contamination puts our water supplies in jeopardy. To help combat this threat, your analysis must be done more reliably, more efficiently, and with higher quality results than ever before.

Whether you need support for a single instrument or a multi-lab, multi-vendor operation, Agilent helps you solve problems quickly, increase your uptime, and optimize your resources – from installation and upgrade to operation and repair.

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With over 100,000 qualification deliveries and decades of quality testing experience, Agilent is a trusted source for system qualification, along with any proof of calibration you might need to comply with regulations.



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You can trust Agilent to help protect your instrument investment today... and transition to next-generation technologies.



"Best in Class" services and support plans:

From service center operations in 65 countries to our global dispatch system to expertly staffed call centers, Agilent provides the personalized support essential to your productivity.

Partnering with you to protect water, health, and quality of life

Organic and inorganic contaminants in water present an ongoing threat to human health – one that underscores the need for fast, dependable analysis.

Agilent has the technology and measurement capabilities you need to ensure the integrity of our water supplies, comply with increasingly strict global regulations, and meet your demands for speed and accuracy.

From determining water purity... to responding to disasters... to identifying emerging contaminants... Agilent helps you increase productivity and generate results with confidence.



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