APPLICATION NOTE 44480

Fast and robust assessment of water quality using ICP-OES

Multielement analysis according to the DIN EN ISO 11885:2009 method requirements

Authors: Sukanya Sengupta[1], Sven Gebhardt[2], and Cristian Cojocariu[3]

[1]Thermo Fisher Scientific, Germany
[2]Niedersächsisches Landesgesundheitsamt, Aurich, Germany
[3]Thermo Fisher Scientific, UK

Keywords: DIN EN/ISO 11885:2009, iCAP PRO Series ICP-OES, ICP-OES, fast analysis, robustness, method validation, sensitivity, limits of quantification, analytical testing, water quality, surface water, drinking water

Goal

To demonstrate the suitability of the Thermo Scientific™ iCAP™ PRO Series ICP-OES for fast, sensitive and robust analysis of major and trace elements in various water samples, including drinking water, following the DIN EN ISO 11885:2009 requirements.

Introduction

Even in small quantities, many elements can have toxic effects when present in drinking supplies or food chains. As such, monitoring the trace elemental composition of drinking, waste, and surface waters (such as rivers, lakes, and ponds) is vital in the maintenance of human, animal, and environmental health. Toxic elements in water, even in small quantities, may end up in the food chain if present in surface waters. Therefore, it is vital that water bodies and drinking waters are regularly checked for their trace elemental composition.

The approach adopted by many nations to ensure water quality is to work to a set of standard guidelines published by a national body. One such body is the Deutsches Institut für Normung - DIN (German Institute for Standardisation), which is the German member body of the International Organization for Standardization (ISO) and is responsible for setting and defining technical standards. ISO sets standards internationally and one such standard, vital for human and environmental health, is the method specified in DIN EN ISO 11885:2009 *Water quality—Determination of selected elements by inductively coupled plasma optical emission spectrometry.*

The DIN EN ISO 11885:2009 method contains performance guidelines and recommends the use of inductively coupled plasma optical emission spectroscopy (ICP-OES) as the analytical instrumentation of choice for assessing both major and trace elements in water samples. ICP-OES instruments are particularly well suited for this analysis as they can effectively perform rapid, low level multielement measurements in a single analytical method (compared to single element techniques such as AAS). However, a common challenge for environmental laboratories analyzing large sample numbers each day is optimizing sample throughput without compromising the sensitivity and productivity, while providing high accuracy, precision, and low limits of detection for key elements.

In this application note, an analytical method using a Thermo Scientific™ iCAP™ PRO Series ICP-OES was developed and validated using multiple systems and various types of waters samples. This study follows the guidelines provided in the DIN EN ISO 11885:2009 method exactly.

Experimental conditions

Instrument parameters for a standard analysis

A Thermo Fisher Scientific™ iCAP™ PRO XP ICP-OES Duo instrument was used for the analysis of trace elemental concentrations in tap, river, and pond water as well as a simulated wastewater matrix. This instrument was selected due to its fully optimizable instrument settings and ability to perform both axial and radial plasma measurements while providing high turnaround. A standard sample introduction kit suitable for aqueous samples was used (Table 1) in conjunction with a Teledyne CETAC™ Technologies ASX-560 autosampler to carry out the analysis. Details of the sample introduction setup and instrument parameters used for the analysis are shown in Table 1 as Method 1.

This method was used to carry out measurements on two different iCAP PRO XP ICP-OES Duo instruments at the Thermo Fisher Scientific facility in Bremen, Germany. The use of two instruments and different measurement days demonstrates the reproducibility, precision, and robustness of the measurements.

Instrument parameters for an enhanced analysis

Additional experiments were performed to enhance sensitivity for certain target elements. For this a U5000AT$^+$ Teledyne CETAC Technologies ultrasonic nebulizer and in-built glass spraychamber were used on an iCAP PRO XP Duo ICP OES instrument at Niedersächsisches Landesgesundheitsamt (State Health Office, Lower Saxony), Aurich, Germany. The method details are listed in Table 1 as Method 2.

Table 1. Instrument configuration and typical operating parameters

iCAP PRO XP Duo parameters		
Parameter	**Method 1 Standard method**	**Method 2 Ultra low detection limit method**
Pump tubing	Sample: Tygon™ orange/white Drain: Tygon white/white	Sample: Tygon white/white Drain: Tygon white/white
Spraychamber	Glass cyclonic	Glass chamber in ultrasonic nebulizer
Nebulizer	Glass concentric nebulizer	U5000AT$^+$ ultrasonic nebulizer, Teledyne CETAC Technologies
Center tube	2.0 mm (quartz)	
Torch	Quartz Duo torch	
Pump speed	45 rpm	75 rpm
Flush pump speed	100 rpm	N.A.
Fast Uptake time/ uptake time	18 s (Fast Uptake)	60 s (no Fast Uptake)
Pump stabilization time	10 s	N.A.
Wash time	25 s	15 s
Nebulizer gas flow	0.65 L·min^{-1}	0.75 L·min^{-1}
Auxiliary gas flow	0.5 L·min^{-1}	
Coolant gas flow	12.5 L·min^{-1}	
RF power	1,150 W	Axial: 1,150 W Radial: 950 W
Radial viewing height	10 mm	12 mm
Repeats	3	
Exposure time	15 s Axial iFR, 5 s Radial iFR	

Sample preparation

The samples used in this study included river water, pond water, and tap water. With the exception of the tap water, the samples were filtered through a 45 µm polycarbonate membrane filter and the filtrates were used for analysis of total dissolved elements in the sample. Nitric acid (TraceMetal™ grade, Fisher Chemical™, US) was added to all samples (final acid concentration in samples 2% (v/v)) to ensure the samples remained stable prior to analysis.

The filters from the pond water filtration samples were digested in a microwave following the digestion procedure described in the DIN EN ISO 11885:2009 method for analyzing particulate matter. For the microwave digestion, 400 mL of the pond water sample was used for filtration and used filters were digested in 9 mL concentrated nitric acid and 1 mL hydrogen peroxide. The final volume recovered after digestion was made up to 50 mL. The sample was then diluted as necessary for the analytes typically expected in high concentrations in such samples.

A solution mimicking a wastewater matrix was prepared in the laboratory for spike recovery tests to demonstrate accuracy in high matrix samples.

Standards

A set of calibration and linearity standards were prepared in 2% (v/v) HNO_3 as listed in Table 2, using certified reference material (CRM) “Multi-element Solution 2” (Sigma-Aldrich™, Sigma-Aldrich Company, UK) and single element solutions (1,000 $mg \cdot L^{-1}$, SPEX CertiPrep™ Group, Metuchen, US).

The DIN EN ISO 11885:2009 method recommends the use of an internal standard to correct for any non-spectral interferences, matrix effects, and signal drift that may occur. Yttrium was used as an internal standard in all samples, calibration, and blank standards that were analyzed using Method 1 to track matrix effects. This was used in the experiments run on the first two instruments.

Table 2. List of target analytes mentioned in DIN EN ISO 11885:2009, calibration standards and linearity ranges

Analyte	Calibration standard 1 ($\mu g \cdot L^{-1}$)	Calibration standard 2 (also used as a QC) ($\mu g \cdot L^{-1}$)	Calibration standard 3 ($\mu g \cdot L^{-1}$)	Calibration standard 4 ($\mu g \cdot L^{-1}$)	Calibration standard 5 ($\mu g \cdot L^{-1}$)
Ag, Al, As, B, Ba, Be, Bi, Cd, Co, Cr, Cu, Fe, Ga, In, Li, Mn, Mo, Ni, P, Pb, S, Sb, Se, Sn, Si, Sr, Ti, U, V, W, Zn, Zr	100	200	500	1,000	–
Ca, Mg, Na, K	100	200	500	1,000	10,000

Quality control

Calibration solution 2 (200 $\mu g \cdot L^{-1}$) (Table 2) was used as a quality control (QC) standard to evaluate analytical precision over time, as advised by the DIN EN ISO 11885:2009 method. Two custom specific CRMs from SCP Science, Canada were also used as QC standards—AQ0-128-151 and AQ0-127-711, their compositions are given in Table 3. The first CRM was diluted 1,000 times to reach a similar concentration to the limit of toxic elements allowed in drinking water in Europe. The second CRM was diluted 100 times to achieve realistic concentrations expected in typical drinking water or tap water. The QC standards were analyzed as a block after every ten samples in every LabBook analyzed during this validation exercise.

Recovery experiments: water spikes

To assess the accuracy of results and their freedom from spectral interferences, the DIN EN ISO 11885:2009 method requires samples to be spiked with known concentration of analytes and these spike recoveries calculated. It is recommended that each sample is spiked with analytes at concentrations of between 10 and 100 times their respective detection limits (element dependent). Following this requirement, the river water and the laboratory simulated wastewater matrix were spiked with the concentrations in Table 4.

Table 3. CRM concentrations after dilution—AQ0-128-151 and AQ0-127-711 (1,000 and 100 times diluted, respectively). The first CRM was diluted 1,000 times to reach the limit of toxic elements allowed in drinking water in Europe.

Analyte	Concentration in AQ0-128-151 (µg·L^{-1})	Concentration in AQ0-127-711 (µg·L^{-1})
Al	200	–
As	10	–
B	1002	–
Cd	4.99	–
Cr	50.1	–
Fe	200.7	–
Mn	503.0	–
Ni	20.04	–
P	10	–
Pb	10	–
Sb	5	–
Se	10	–
U	10	–
Zn	502	–
Ca	–	25,030
Cu	–	2,000
K	–	7,490
Mg	–	11,930
Na	–	24,870

Table 4. Spiked amounts in water samples

Analyte	Spiked amounts (µg·L^{-1})	
	River water sample	Wastewater matrix
Ba, Be, Mn, Sr, Ti	0.5	5
Al, Cd, Co, Cr, Cu, Ga, Mg, Mo, Mn, Ni, V, Zn, Zr	5	5
Ag, As, B, Ca, Fe, In, Li, P, Pb, S, Sb, Si, Sn, Sr, U, W	50	50
S, Si, K, Na	1,000	1,000

Data acquisition and data processing

The Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software was used to create LabBooks for sample analysis, data acquisition, processing, and reporting.

Results and discussion

To check the suitability of this analytical setup for water quality assessment according to the DIN EN ISO 11885:2009 method, the following evaluations were performed on two separate instruments:

- Sensitivity (limit of detection X_{LD}, limit of quantification X_{LQ})
- Linearity
- Accuracy
- Matrix effects and interference removal
- Validation of method using real samples for analytical testing (robustness of method)

Wavelength selection

Wavelengths with high intensities and interference free spectra were chosen for the analytes. A small number of occasional interferences observed were resolved by selecting interference-free integration positions in the respective subarrays. A list of the wavelengths with best detection limits is given in Table 5. The list of recommended wavelengths in the DIN EN ISO 11885:2009 method was used as a guideline.

Sensitivity

Method sensitivity was tested by determining the limit of detection (X_{LD}) and the limit of quantification (X_{LQ}) for target elements. These terms are defined in the DIN EN ISO 11885:2009 as given in Equation 1 and Equation 2.

The limit of detection or X_{LD} is defined in the DIN EN ISO 11885:2009 method as the smallest amount or concentration of an analyte in the test sample that can be reliably distinguished from zero. The X_{LD} for each analyte is determined as in Equation 1, where s_0 is the standard deviation of the concentration of three measurements of the calibration blank with each blank described as “Average Blank” in the Sample List section of the Qtegra ISDS Software LabBook. The X_{LD} values are calculated by Qtegra ISDS Software for each analyte, per wavelength and view.

Equation 1

$$X_{LD} = 3\ s_0$$

The limit of quantification is defined as the smallest amount or concentration of an analyte in the test sample that can be determined with a fixed precision. It is calculated as below in Equation 2. The X_{LQ} values achieved for all analytes were better than required in the DIN EN ISO 11885 method and are listed in Table 5.

Equation 2

$$X_{LQ} = 3\ X_{LD} = 9\ s_0$$

The X_{LD} values obtained in this study using the concentric glass nebulizer and glass cyclonic spray chamber are all in the single digit µg·L^{-1} (ppb) range and the requirements of the DIN EN ISO 11885:2009 are met for each analyte (Table 5). The DIN EN ISO 11885:2009 method provides an estimate of the achievable X_{LD} based on interlaboratory trial, and the limits achieved in the current study by analysis on three different instruments and two laboratories are well below those values.

To achieve even lower detection limits and limits of quantification, an ultrasonic nebulizer (USN) with in-built spraychamber was used in combination with the iCAP PRO XP ICP-OES Duo instrument in this study (Table 1, Method 2). This setup yields several times lower detection limits and is a cost-effective solution for laboratories seeking to detect ultra-low levels of analytes in drinking water samples. Table 6 shows the achievable improved detection limits for some important elements, critical for drinking water analysis, with the use of the USN.

Table 5. List of best wavelengths, corresponding limits of detections (X_{LD}) and limits of quantification (X_{LQ}) for analytes included in the DIN EN ISO 11885 method for water quality determination using glass concentric nebulizer. Multiple wavelengths were verified as suitable wavelengths for this type of analysis for most analytes but the ones with best sensitivities and lowest X_{LD} and X_{LQ} are listed here.

Analyte	Wavelength (nm)	Viewing mode, all iFR	X_{LD} (µg·L^{-1})	X_{LQ} (µg·L^{-1})
Ag	328.068	Axial	0.87	2.61
Al	167.079	Axial	0.14	0.42
As	189.042	Axial	1.48	4.44
B	249.773	Axial	0.71	2.13
Ba	233.527	Axial	0.06	0.18
Be	234.861	Axial	0.03	0.09
Bi	223.061	Axial	0.84	2.52
Ca	315.887	Radial	2.93	8.79
Cd	214.438	Axial	0.09	0.27
Co	228.616	Axial	0.16	0.48
Cr	267.716	Axial	0.09	0.27
Cu	324.754	Axial	0.22	0.66
Fe	238.204	Axial	0.11	0.33
Ga	287.424	Axial	1.21	3.63
In	325.609	Axial	2.58	7.74
K	766.490	Radial	13.0	39.0
Li	670.791	Radial	0.58	1.74
Mg	279.553	Radial	0.13	0.39
Mn	257.610	Axial	0.003	0.009
Mo	202.030	Axial	0.43	1.29
Na	589.592	Radial	5.19	15.57
Ni	231.604	Axial	0.6	1.8
P	177.495	Axial	1.54	4.62
Pb	220.353	Axial	0.83	2.49
S	180.731	Axial	1.68	5.04
Sb	206.833	Axial	1.18	3.54
Se	196.09	Axial	2.29	6.87
Si	212.412	Axial	1.67	5.01
Sn	189.989	Axial	0.74	2.22
Sr	407.771	Axial	0.01	0.03
Ti	334.941	Axial	0.04	0.12
U	367.007	Axial	1.65	4.95
V	290.882	Axial	0.87	2.61
W	207.911	Axial	0.5	1.5
Zn	206.200	Axial	0.37	1.11
Zr	339.198	Axial	0.07	0.21

Table 6. Improved X_{LD} and X_{LQ} obtained by using the ultrasonic nebulizer (USN), of some important analytes that are critical for drinking water analysis

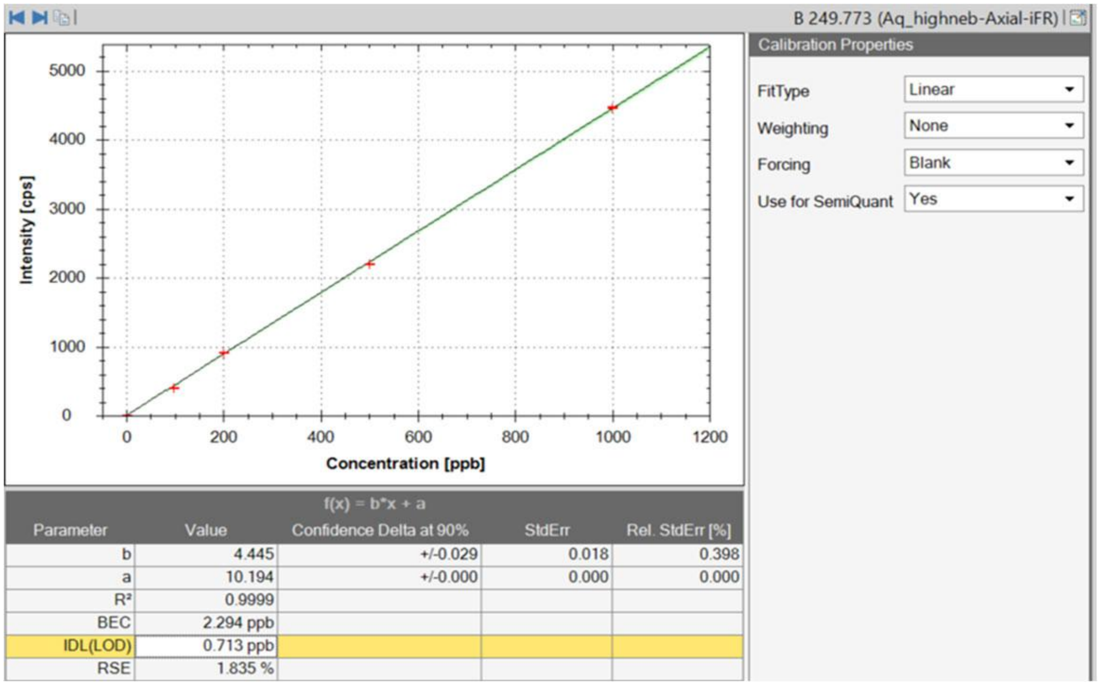
Analyte	Wavelength (nm)	Viewing mode, all iFR	X_{LD} (µg·L^{-1}) achievable with the USN for best wavelengths	X_{LQ} (µg·L^{-1}) achievable with the USN for best wavelengths	Improvement factor compared to normal glass nebulizer
As	189.042	Axial	0.40	1.2	3.7
Be	234.861	Axial	0.01	0.03	3.0
Cd	214.438	Axial	0.02	0.06	4.5
Ga	287.424	Axial	0.08	0.24	15.1
In	325.609	Axial	0.77	2.31	3.4
Mg	279.553	Radial	0.03	0.09	4.3
Mo	202.030	Axial	0.04	0.12	10.8
Pb	220.353	Axial	0.19	0.57	4.4
Sb	206.833	Axial	0.28	0.84	4.2
Sn	189.989	Axial	0.15	0.45	4.9
U	409.014	Axial	1.14	3.42	3.5
V	290.882	Axial	0.17	0.51	5.1

Linearity

The calibration curves for the different wavelengths gave R^2 values greater than 0.9997 over a calibration range of 0–10,000 µg·L^{-1} for alkali elements and up to 1,000 µg·L^{-1} for other analytes (example of a calibration curve in Figure 1).

Accuracy

The DIN EN ISO 11885:2009 method requires recoveries of concentrations of spiked amounts to be within ±20% of the known value that was added. Most recoveries in this study were in the ±15% range with some exceptions but all analytes recoveries were within the ±20% acceptable interval Figure 2.



B 249.773 (Aq_highneb-Axial-iFR)

Calibration Properties

FitType: Linear
Weighting: None
Forcing: Blank
Use for SemiQuant: Yes

f(x) = b*x + a

Parameter	Value	Confidence Delta at 90%	StdErr	Rel. StdErr [%]
b	4.445	+/-0.029	0.018	0.398
a	10.194	+/-0.000	0.000	0.000
R²	0.9999			
BEC	2.294 ppb			
IDL(LOD)	0.713 ppb			
RSE	1.835 %			

Figure 1. Calibration curve for B 249.773 nm in Axial viewing mode. This is found under the Concentrations section in the Qtegra ISDS Software LabBook and below this plot the limit of detection (X_{LD} as IDL) is displayed.

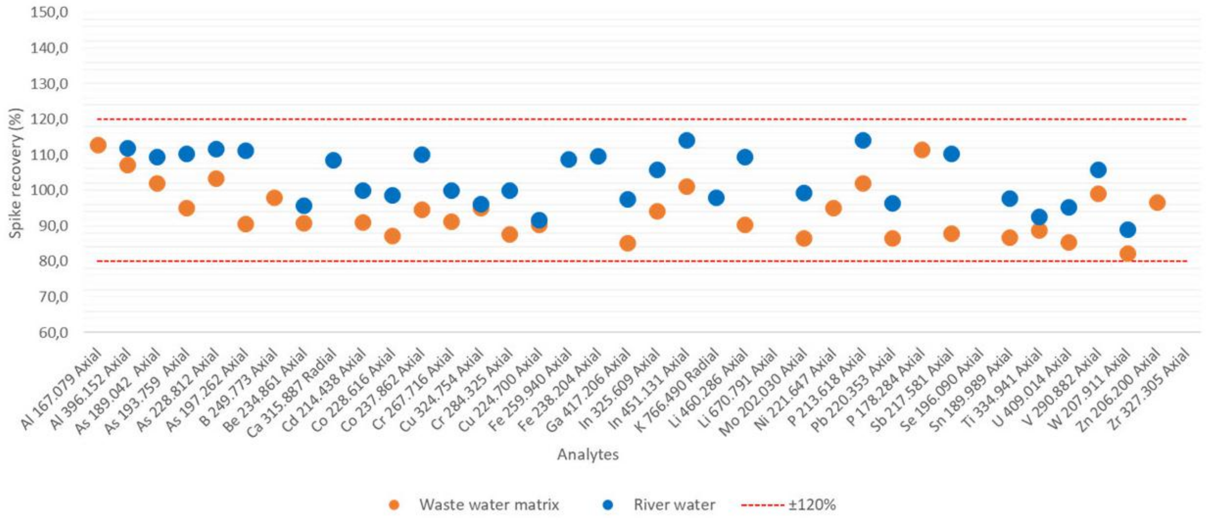


Figure 2. Spike recoveries in river water sample and laboratory simulated wastewater matrix. The dashed line represents the maximum allowed recovery interval (± 20%) as specified in the DIN EN ISO 11885:2009 method.

Matrix effects and non-spectral interferences

Recovery of the internal standard was between 80 and 110% over the entire duration of the experiments and in all different types of sample matrices, demonstrating no matrix suppression / enhancement effects or non-spectral interference, thereby further ensuring the data accuracy (Figure 3).

Robustness

Measurements were run to test the applicability of the developed method in analytical testing laboratories for daily sample analysis. Three stability tests were performed for this study using the method parameters described in Table 1. Method 1 from Table 1 was performed on two different iCAP PRO XP ICP-OES Duo instruments at the Thermo Fisher Scientific laboratory in Bremen, Germany. The third was performed in the laboratory of Niedersächsisches Landesgesundheitsamt, Aurich, Germany, using Method 2 from Table 1, i.e., using an ultrasonic nebulizer (USN).

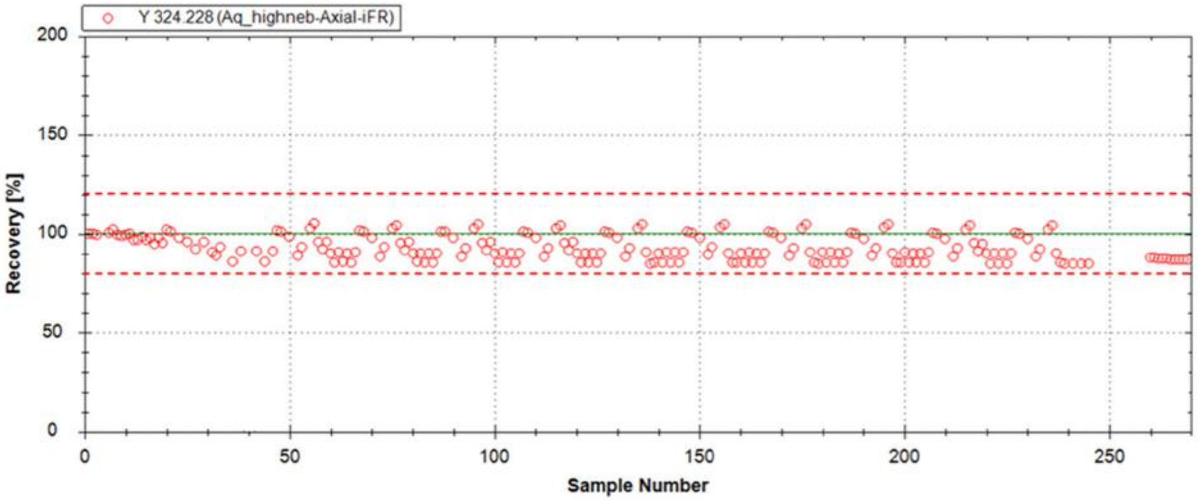


Figure 3. Example of internal standard recovery in Axial mode on Instrument 1

Each stability test was started with at least three blank measurements, followed by calibration standards, then analysis of the highest standard as an unknown sample (where the resulting concentration was within ±5% of expected value), QCs (Table 2, Table 3), and finally samples, as described in the DIN EN ISO 11885:2009 method. All three QCs were run every 10 samples to ensure accuracy and precision over long analysis times.

All three instruments were found to perform comparably in terms of signal stability and reproducibility over a typical working day. The analyte recoveries of two CRMs and calibration standard 2 (used as a QC) was between 80 and 120% over 8 hours of long-term analyses (Figure 4, Figure 5, and Figure 6). The recoveries of concentrations of the river water sample during the stability experiments on the instruments was within 90–110% (Figure 7).

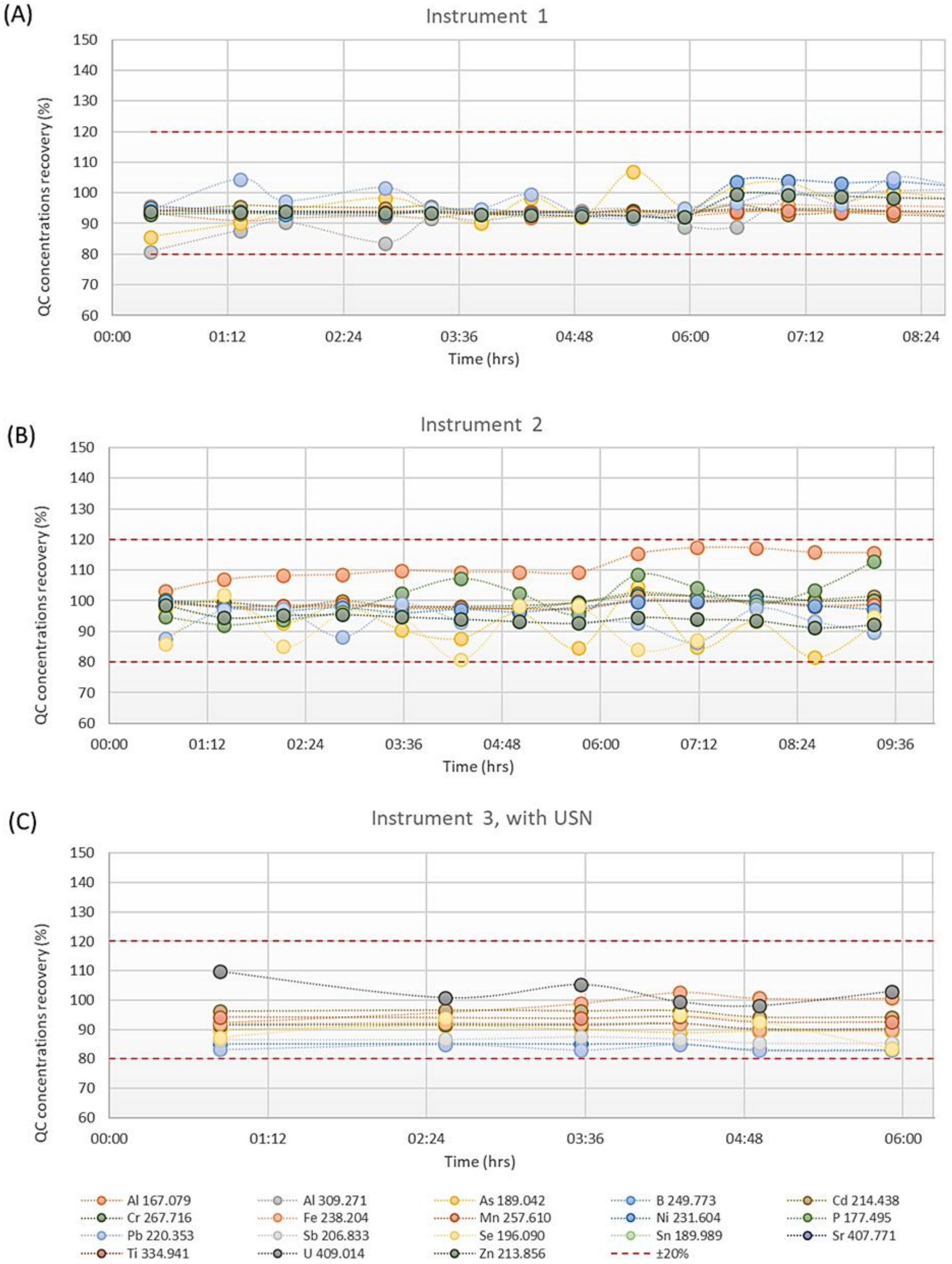


Figure 4. Long-term experiments demonstrating recoveries of target elements in the QC standard AQO-128-151, 1,000x diluted, data obtained on three distinct iCAP PRO XP ICP-OES Duo systems. The dashed line represents the maximum allowed recovery interval (± 20%) as specified in the DIN EN ISO 11885:2009 method. Additional experiments using the USN (panel C) were run in the customer laboratory where a smaller number of measurements were made.

Short exposure times of 15 s in Axial iFR mode and 5 s in Radial iFR mode provided excellent detection limits on all analytes (Table 5). Since all wavelengths could be analyzed simultaneously in a single mode, the run time per sample was only 2 minutes 20 seconds, including sample uptake, measurement, and rinse.

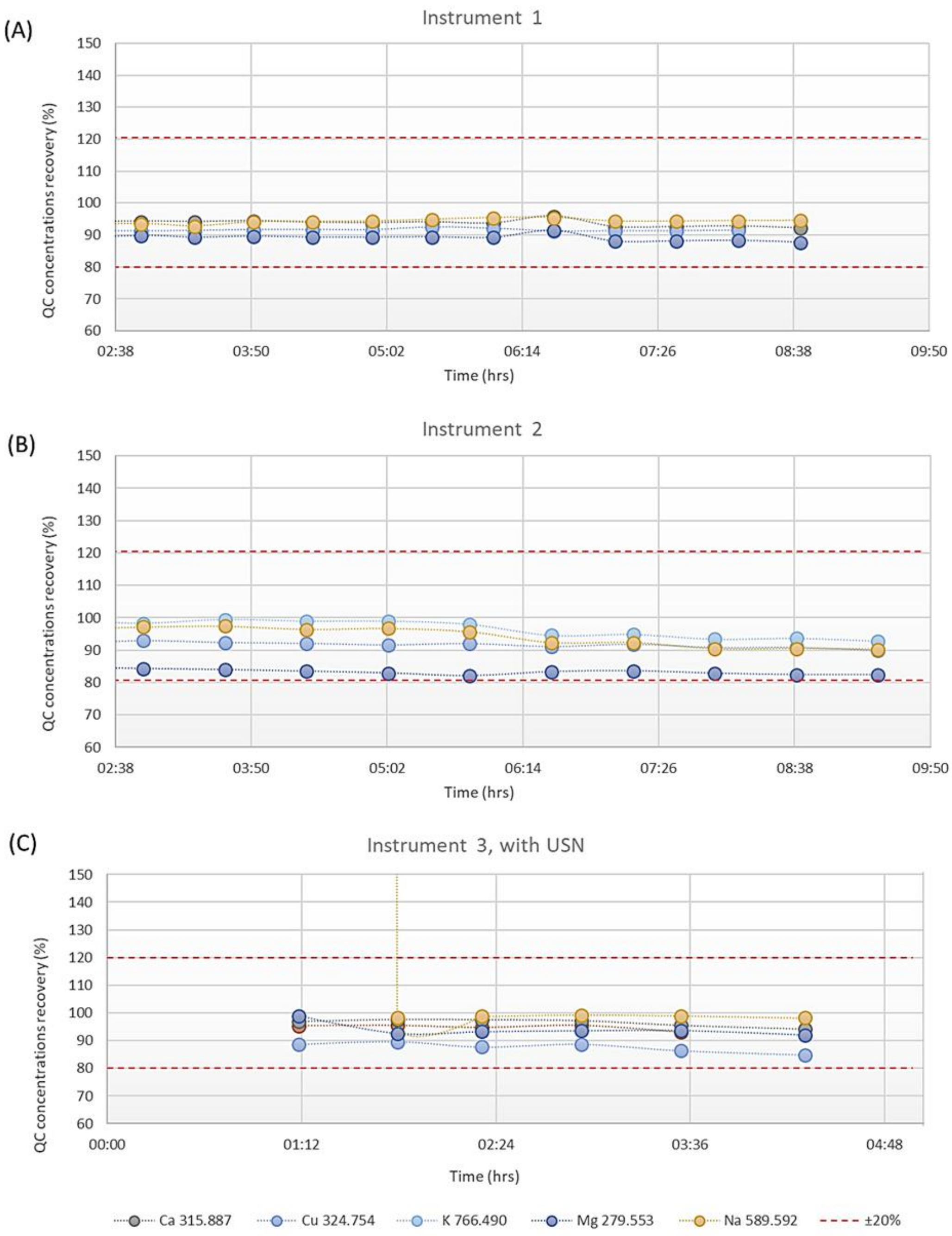


Figure 5. QC standard recoveries of AQO-127-711, 100x diluted, in stability experiments on three different iCAP PRO XP ICP-OES Duo systems. The dashed line represents the maximum allowed recovery interval (±20%) as specified in the DIN EN ISO 11885:2009 method. Additional experiments using the USN (panel C) were run in the customer laboratory where a smaller number of measurements were made.

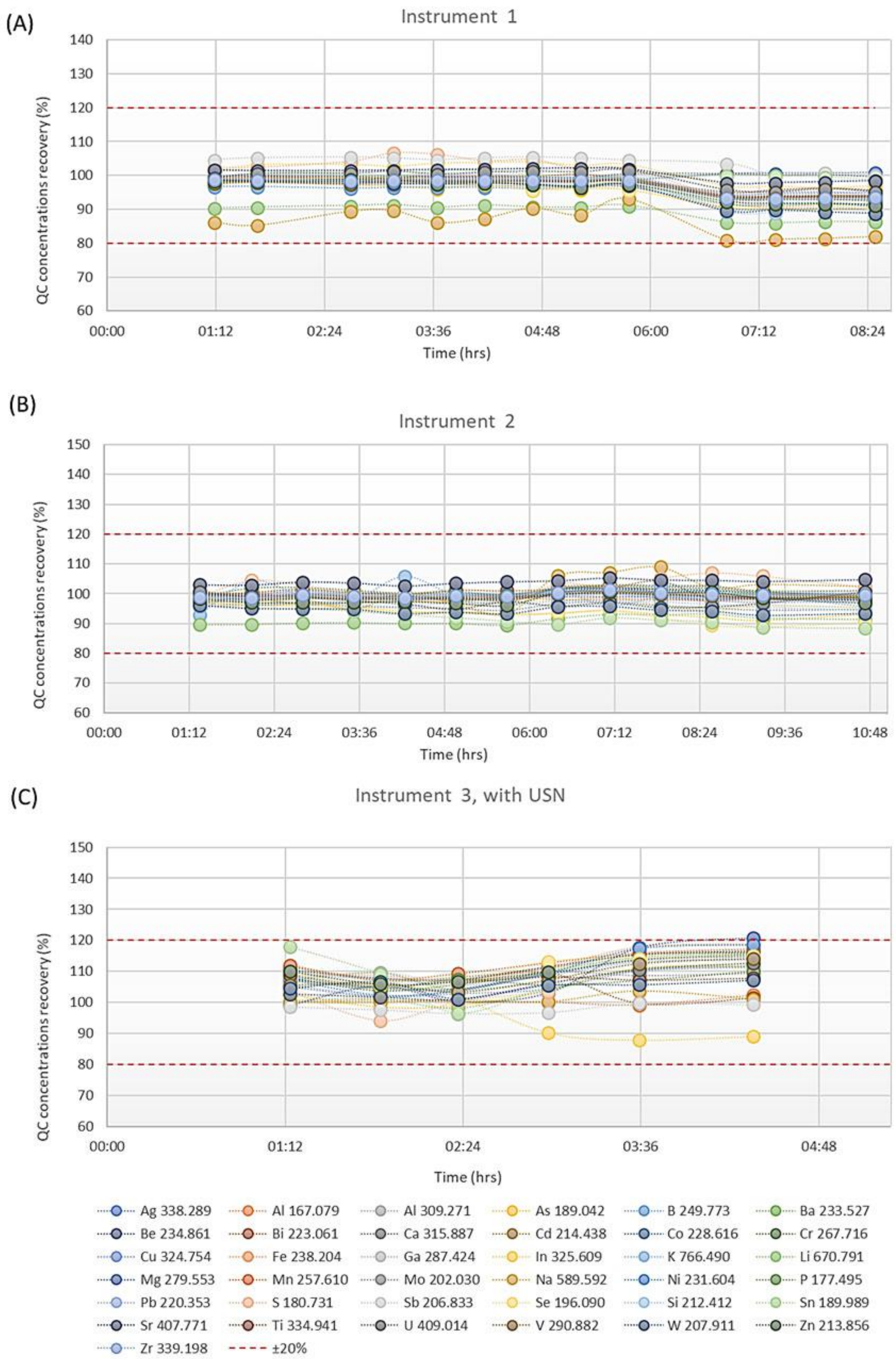


Figure 6. Recoveries of analytes present in calibration standard 2 (200 µg·L^{-1}) used as a QC standard and analyzed every 10 water samples to demonstrate accuracy and repeatability of all analytes included in DIN EN ISO 11885:2009 method. This data was obtained from three different iCAP PRO XP ICP-OES Duo systems (the number of measurements was smaller in panel C as this was performed in customer laboratory). The dashed line represents the maximum allowed recovery interval (±20%) as specified in the DIN EN ISO 11885:2009 method.

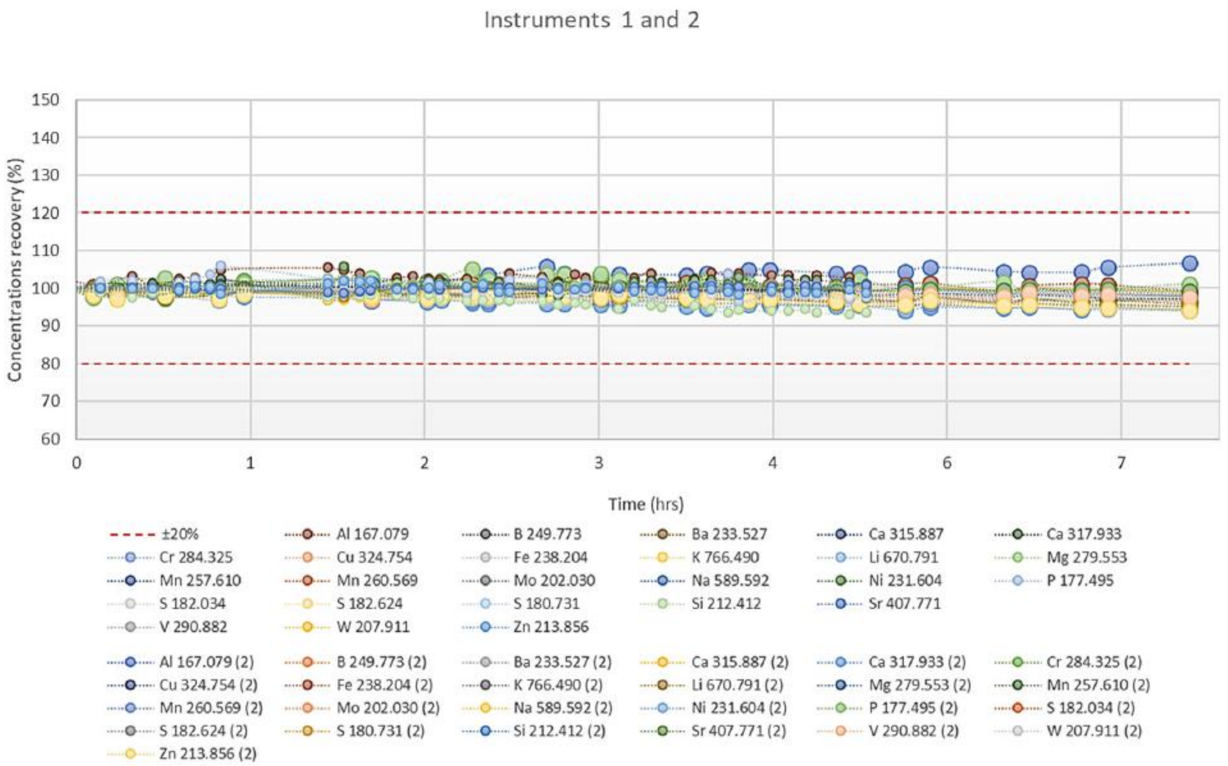


Figure 7. Recoveries of analyte concentrations in river water samples, as given in Table 8, displaying the stability performance of the two different iCAP PRO XP ICP-OES Duo systems—instruments 1 (small circles) and 2 (big circles)—over several hours of uninterrupted analysis of water samples. The time axis starts with the first measurement of the sample and does not include the time taken to run the calibration block of the day.

Table 7. Particulate trace elemental composition of the pond water sample. Measured samples were eight times more concentrated relative to the original sample volume.

Analyte and wavelength (nm)	Concentrations (µg·L^{-1})
Ag 338.289	<DL
Al 167.079	143.4
As 189.042	<DL
B 249.773	<DL
Ba 455.403	0.8
Be 313.042	<DL
Bi 223.061	<DL
Ca 315.887	30.3
Cd 214.438	<DL
Co 238.892	<DL
Cu 324.754	7.1
Cr 283.563	<DL
Fe 238.204	63.7
Ga 294.364	<DL
In 325.609	<DL
K 766.490	57.8
Mg 279.553	20.9
Mn 257.610	0.3
Mo 202.030	<DL
Na 589.592	16.8
Ni 231.604	<DL
P 177.495	3.2
Pb 220.353	<DL
Sb 217.581	<DL
Se 196.090	<DL
S 180.731	15.1
Si 212.412	457.1
Sn 189.989	<DL
Sr 407.771	0.2
Ti 334.941	8.8
U 367.007	<DL
V 309.311	<DL
W 239.709	<DL
Zn 213.856	<DL
Zr 339.198	0.4

The concentration of particulate matter in the pond water sample is given in Table 7. These values are relevant for studies where total composition of the sample is of interest—both dissolved elements (Figure 8 in main text; Table 9 and Table 10 in Appendix) and those present within the undissolved particulate fraction of the samples.

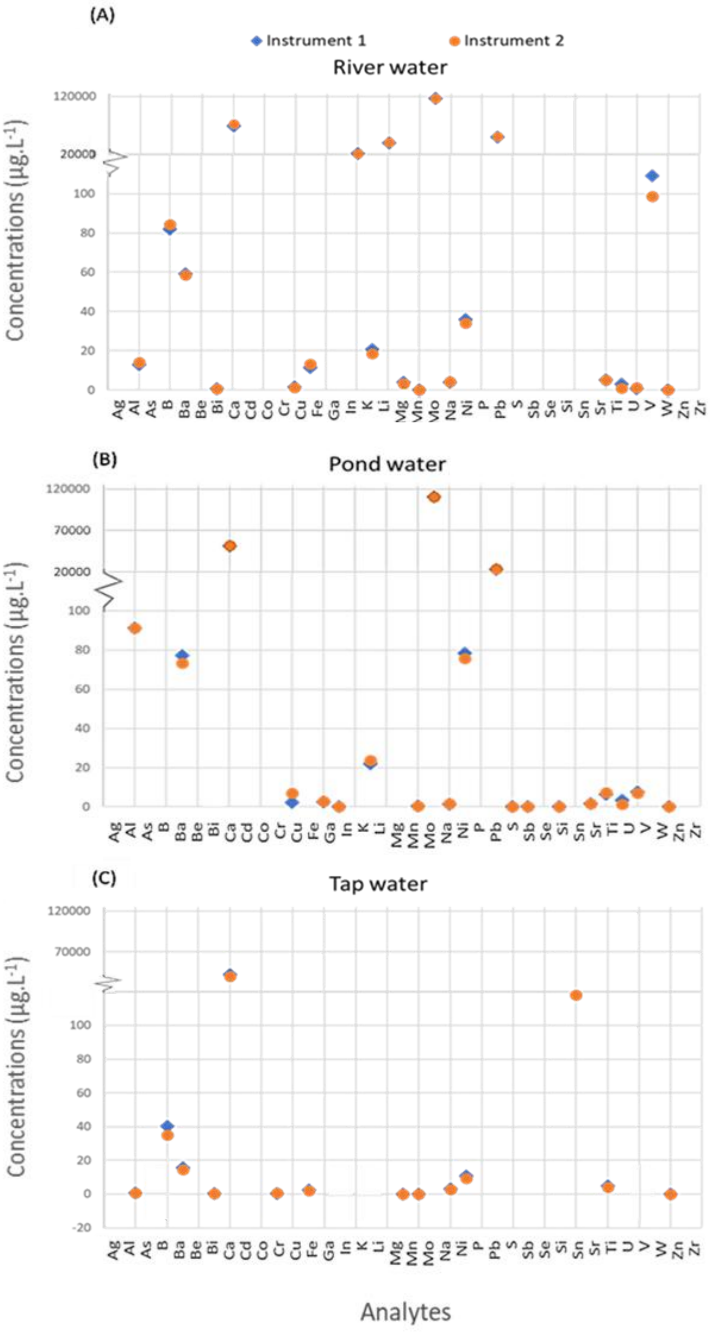


Figure 8. Plots comparing the dissolved trace elemental composition of river water, pond water, and tap water samples from three different instruments.

Conclusions

This application note demonstrates the suitability of the iCAP PRO XP ICP-OES Duo instrument for water analysis according to the requirements and guidelines described in the DIN EN ISO 11885:2009 method. Fast, highly sensitive, reliable, and robust analysis of different kinds of water sample types was achieved with the use of three different iCAP PRO XP ICP-OES Duo instruments in two different laboratories, demonstrating the excellent data reproducibility, reliability, and robustness of the instruments.

- Wide linear dynamic ranges were achieved for all target elements mentioned within the scope of the DIN EN ISO 11885 method; 0 to 1,000 µg·L^{-1} was obtained for most analytes and higher levels of up to at least 10,000 µg·L^{-1} (in radial mode) was achieved for major elements, proving the suitability of the iCAP PRO XP ICP-OES for detecting a variety of elements in varied concentrations in water samples. This was consistent over the three different instruments and completely fulfils the requirements of the DIN EN ISO 11885:2009 method.
- The iCAP PRO XP ICP-OES offers the flexibility to choose analytical wavelengths to be used, depending on the expected element concentrations and presence of potential interferences. The wavelengths fit for use in water samples were characterized, with the optimal ones determined for the method detailed above.
- Sensitivity in the ppt level for 75% of the target analytes and low ppb level for the remaining 25% of the analytes was achieved with a normal glass nebulizer. The requirements of the DIN EN ISO 11885 method were fully satisfied and exceeded in many cases.
- Even lower detection limits and higher sensitivity are achievable by coupling the iCAP PRO XP ICP-OES Duo to an ultrasonic nebulizer (USN) in the case it is necessary to measure low ppb level concentrations required to meet drinking water regulations.
- Two CRMs were run successfully during long-term experiments and excellent accuracy was obtained for the analytes against certified concentrations, demonstrating the signal stability and robustness of the iCAP PRO XP Duo ICP-OES over time.

- Recovery values within the expected (±20%) range were obtained for spiked samples, demonstrating the accuracy of the technique and analytical setup.
- Excellent system robustness, inter-laboratory accuracy, and reproducibility were demonstrated from three experiments performed on three different iCAP PRO XP ICP-OES Duo instruments in two different laboratories.
- Fast analysis for all target analytes utilizing both Axial and Radial modes (2 min 20 s per sample) was achieved with this multi-element method. This enabled high sample throughput with minimal downtime, requiring no user interaction required for long time periods. This is especially important for analytical testing laboratories where hundreds of samples may need to be analyzed daily.

Reference

1. DIN EN ISO 11885:2009—Water quality—*Determination of selected elements by inductively coupled plasma optical emission spectrometry* (ICP-OES) (ISO 11885:2007); German version EN ISO 11885:2009. German title—*Wasserbeschaffenheit—Bestimmung von ausgewählten Elementen durch induktiv gekoppelte Plasma-Atom-Emissionsspektrometrie* (ICP-OES) (ISO 11885:2007); Deutsche Fassung EN ISO 11885:2009. Publication date—**2009-09**. Original language—German.

Appendix

This appendix presents data on dissolved trace elemental composition of a different water samples analyzed in the present study using two different iCAP PRO XP ICP-OES Duo instruments. These data have been plotted in Figure 8 in the main text of the application note.

Table 8. Consistency of results as demonstrated for dissolved trace elements concentrations in a river water sample analyzed on two different iCAP PRO XP ICP-OES Duo systems

Sample	Concentrations in the river water sample (µg·L^{-1})	
Analytes and wavelengths (nm)	Instrument 1	Instrument 2
Ag 328.068	<DL	<DL
Al 167.079	12.9	14.2
As 189.042	<DL	<DL
B 249.773	82.3	84.8
Ba 233.527	59.7	58.8
Be 234.861	<DL	<DL
Bi 223.061	0.5	0.6
Ca 315.887	70,338.1	72,597.2
Cd 214.438	<DL	<DL
Co 228.616	<DL	<DL
Cr 283.563	<DL	<DL
Cu 324.754	1.6	1.2
Fe 238.204	11.4	13.1
Ga 287.424	<DL	<DL
In 325.609	<DL	<DL
K 766.490	22,267.4	22,603.4
Li 670.791	20.7	18.7
Mg 279.079	40,790.0	41,566.5
Mn 257.610	3.9	3.4
Mo 202.030	<DL	<DL
Na 589.592	117,837.5	117,684.6
Ni 231.604	3.9	4.1
P 177.495	36.2	34.3
Pb 220.353	<DL	<DL
S 180.731	50409.5	51431.4
Sb 206.833	<DL	<DL
Se 196.090	<DL	<DL
Si 212.412	232.0	221.0
Sn 189.989	<DL	<DL
Sr 407.771	692.0	624.5
Ti 334.941	<DL	<DL
U 367.007	5.0	5.2
V 290.882	<DL	<DL
W 207.911	<DL	<DL
Zn 213.856	109.5	99.0
Zr 339.198	<DL	<DL

Table 9. Dissolved trace elements concentrations in the pond water sample on two different iCAP PRO XP ICP-OES Duo systems

Sample	Concentrations in pond water sample (µg·L^{-1})	
Analytes and wavelengths (nm)	Instrument 1	Instrument 2
Ag 328.068	<DL	<DL
Al 167.079	91.2	91.3
As 189.042	<DL	<DL
B 249.773	135.7	139.2
Ba 233.527	77.2	73.4
Be 234.861	<DL	<DL
Bi 223.061	<DL	<DL
Ca 315.887	51,298.0	51,969.6
Cd 214.438	<DL	<DL
Co 228.616	<DL	<DL
Cr 283.563	<DL	<DL
Cu 324.754	2.3	6.9
Fe 238.204	858.0	717.2
Ga 287.424	2.7	2.8
In 325.609	<DL	<DL
K 766.490	8,578.2	7,769.10
Li 670.791	22.1	23.8
Mg 279.079	9,338.6	8,486.7
Mn 257.610	705.3	578.6
Mo 202.030	<DL	<DL
Na 589.592	110,698.5	110,374.3
Ni 231.604	1.3	1.5
P 177.495	78.6	75.8
Pb 220.353	<DL	<DL
S 180.731	22,907.3	23,311.0
Sb 206.833	<DL	<DL
Se 196.090	<DL	<DL
Si 212.412	7,217.2	7,282.0
Sn 189.989	<DL	<DL
Sr 407.771	355.2	300.7
Ti 334.941	1.7	1.6
U 367.007	6.5	7.4
V 290.882	<DL	<DL
W 207.911	7.5	6.9
Zn 213.856	881.2	811.2
Zr 339.198	<DL	<DL

Table 10. Dissolved trace elements concentrations of tap water sample on two different iCAP PRO XP ICP-OES Duo systems

Sample	Concentrations in tap water sample (µg·L^{-1})	
Analytes and wavelengths (nm)	Instrument 1	Instrument 2
Ag 328.068	<DL	<DL
Al 167.079	0.6	0.7
As 189.042	<DL	<DL
B 249.773	40.4	35.2
Ba 233.527	15.8	14.6
Be 234.861	<DL	<DL
Bi 223.061	0.5	0.4
Ca 315.887	41,619.9	39,576.1
Cd 214.438	<DL	<DL
Co 228.616	<DL	<DL
Cr 283.563	0.3	0.7
Cu 324.754	142.6	138.0
Fe 238.204	2.5	2.0
Ga 287.424	<DL	<DL
In 325.609	<DL	<DL
K 766.490	2,560.1	2,675.4
Li 670.791	<DL	<DL
Mg 279.079	3766.9	3617.5
Mn 257.610	0.2	<DL
Mo 202.030	<DL	<DL
Na 589.592	13,814.2	12,241.3
Ni 231.604	3.0	2.7
P 177.495	10.7	9.4
Pb 220.353	<DL	<DL
S 180.731	12,111.4	11,261.3
Sb 206.833	<DL	<DL
Se 196.090	<DL	<DL
Si 212.412	8,852.3	8,758.6
Sn 189.989	<DL	<DL
Sr 407.771	127.8	118.0
Ti 334.941	<DL	<DL
U 367.007	5.0	4.1
V 290.882	<DL	<DL
W 207.911	2.1	3.0
Zn 213.856	295.2	328.6
Zr 339.198	<DL	<DL

Find out more at **thermofisher.com/icp-oes**