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Getting the Most from Your Laboratory Provider: Assuring Defensible Decisions in Water Testing

Presented by Prianshu Chawla



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WARNING!

Please limit to 15 kg
to avoid back injury.



Topics

- The Water Testing Journey: From Sampling to Reported Result
- Analytical Method Measurement of Uncertainty: From Validation to Result Interpretation
- QA/QC as the Foundation of Reliable Results

Typical Laboratory 'Jargon'



- SRN/SRA, COA, COC, QA/QC interpretive reports, EDD's
- Suites or Packages
- LOR, MDL
- UT, LL, ST
- Spikes (matrix vs. surrogate), RPDs, Blanks
- LCS
- MB

PFAS Water Analytical Testing Roadmap



Extraction

Concentrating sample using SPE to reach part-per-trillion (ppt) detection levels.



Analysis

Triple Quadrupole LC-MS/MS



Review

Data review ensuring Isotope Dilution recoveries and QA/QC meet method limits.

First Step in Defensible Data - Representative Water Sampling



- Laboratories request extra containers to ensure technical reserve or immediate re-analysis if instrument issues occur.
- While three are provided, the lab typically uses **only one container** for the primary extraction process
- Because only a portion of the total volume is tested, field sampling must ensure the water is representative of the source.

PFAS Sample Extraction - Solid Phase Extraction (SPE)

Cartridge Loading: Passing the sample through a sorbent bed to selectively bind PFAS molecules.

Matrix Cleanup: Washing away interfering salts and organic matter.

Elution: Using organic solvents to release the target analytes for instrumentation.



Low Level Results Need High Level Confidence



- After extraction, the sample is introduced into LC-MS/MS for compound specific measurement.
- Before reporting, the laboratory reviews the data to confirm that the result can be supported with confidence.



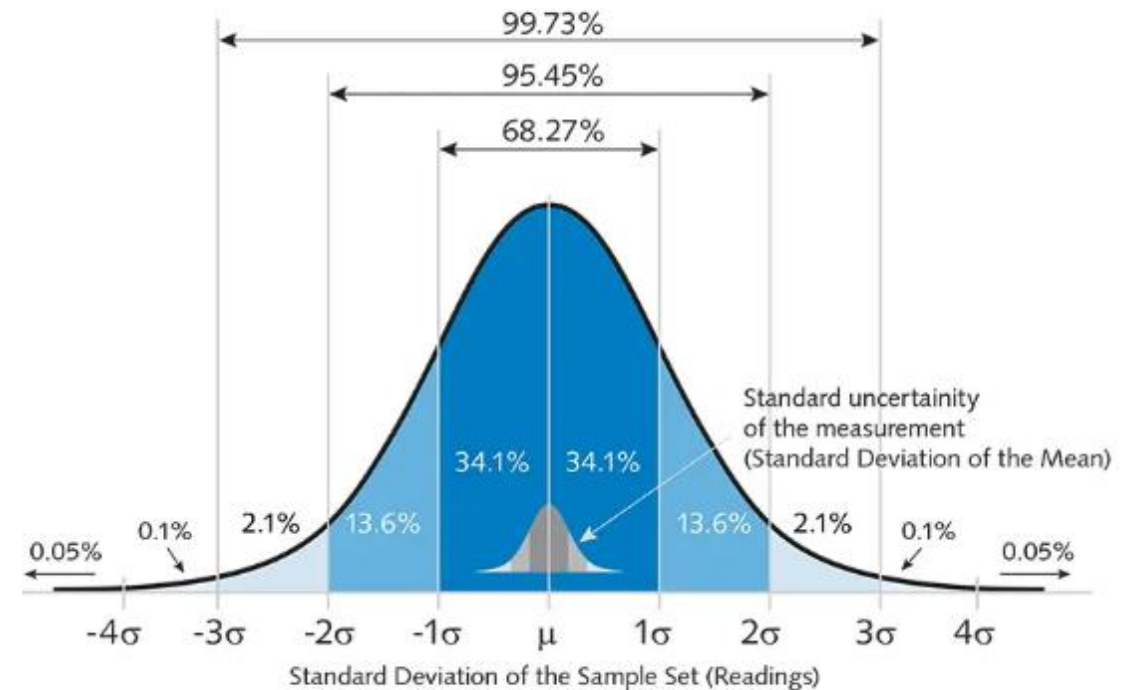
Why the Range Around a Number Matters



Uncertainty is not "Error". It is a statistical range where the true value resides with high confidence.
Support interpretation near Reporting Limit (RL)

Statistical Basis

Calculated using a coverage factor ($k=2$), providing a 95% confidence interval for every reported result.





From Precision Data to an Initial Uncertainty Estimate

The uncertainty % is scientifically derived from a method validation dataset

Source of Variance	Description
Calibration Standards	Uncertainty reported on the certificate of the CRM.
Instrumental Precision	Statistical variance across multiple analytical injections.
Sample Preparation	Variability introduced during pipetting and extraction steps.
Matrix Effects	Suppression or enhancement caused by unique water chemistry.



Interpreting Results Close to the Reporting Limit

Parameter	Value
Reporting Limit (RL)	1.0 ng/L
Reported Result	1.1 ng/L
Method Uncertainty	± 22%
Uncertainty Range	0.86 – 1.34 ng/L

A result near the RL should be interpreted as a low-level detected value with appropriate uncertainty context, rather than relying on the single reported number.

Understanding the ALS UoM Report



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Analytical Results

Sub-Matrix: WASTE WATER
(Matrix: WATER)

				Client Sample ID	Test Water 1	Test Water 2	Test Water 3	Test Water 4	Test Water Fail
				Client Sampling date / time	13-Apr-2026 10:00	13-Apr-2026 10:00	13-Apr-2026 10:00	13-Apr-2026 10:00	13-Apr-2026 10:00
Compound	CAS Number	LOR	Unit		NH2601573-001	NH2601573-002	NH2601573-003	NH2601573-004	NH2601573-005
					Result UOM	Result UOM	Result UOM	Result UOM	Result UOM
HMSol_W: Elements in Water (Soluble)									
Aluminium	7429-90-5	0.003	g/m3		1.00 ± 30.0%	----	----	----	----
Antimony	7440-36-0	0.0001	g/m3		1.00 ± 30.0%	----	----	----	----
Arsenic	7440-38-2	0.0005	g/m3		1.00 ± 30.0%	----	----	----	----
Barium	7440-39-3	0.0002	g/m3		1.00 ± 30.0%	----	----	----	----
Beryllium	7440-41-7	0.00001	g/m3		1.00 ± 30.0%	----	----	----	----
Bismuth	7440-69-9	0.0001	g/m3		1.00 ± 30.0%	----	----	----	----
Boron	7440-42-8	0.01	g/m3		1.00 ± 30.0%	----	----	----	----
Cadmium	7440-43-9	0.00002	g/m3		1.00 ± 30.0%	----	----	----	----
Caesium	7440-46-2	0.00001	g/m3		1.00 ± 30.0%	----	----	----	----
Calcium	7440-70-2	0.05	g/m3		1.00 ± 10.0%	----	----	----	----
Chromium	7440-47-3	0.0002	g/m3		1.00 ± 30.0%	----	----	----	----
Cobalt	7440-48-4	0.00001	g/m3		1.00 ± 30.0%	----	----	----	----
Copper	7440-50-8	0.0002	g/m3		1.00 ± 30.0%	----	----	----	----
Germanium	7440-56-4	0.00005	g/m3		1.00 ± 30.0%	----	----	----	----
Iron	7439-89-6	0.005	g/m3		1.00 ± 30.0%	----	----	----	----
Lanthanum	7439-91-0	0.00001	g/m3		1.00 ± 30.0%	----	----	----	----
Lead	7439-92-1	0.00005	g/m3		1.00 ± 30.0%	----	----	----	----
Lithium	7439-93-2	0.00001	g/m3		1.00 ± 30.0%	----	----	----	----

QA/QC



QA – quality assurance

&

QC – quality control

=

Confidence

Note: the quality of the analysis is only as good as the quality of the sample taken.



What is QA/QC?

- QA (Quality Assurance) and QC (Quality Control) are the processes used to measure the quality of our testing.
- 6 major parameters
 - Blanks (five types)
 - Duplicates (two types)
 - Lab Control Samples
 - Matrix Spikes
 - Surrogates
 - Trip Spikes

Important term – Analytical Runs

	Cup #	Qc Type	Sample Type	Sequence
>	1	BLK	MB	1
	2	STD	LCS	1
	3	REG	REG	1
	4	DUP	DUP	1
	5	SPK	MS	1
	6	REG	REG	1
	7	REG	REG	1
	8	REG	REG	1
	9	REG	REG	1
	10	REG	REG	1
	11	REG	REG	1
	12	REG	REG	1
	13	REG	REG	1
	14	REG	REG	1
	15	REG	REG	1
	16	DUP	DUP	1
	17	REG	REG	1
	18	REG	REG	1
	19	REG	REG	1
	20	REG	REG	1

— Method Blank: 1 in 20

— Lab Control Sample: 1 in 20

— Duplicates: 1 in 10

— Matrix Spike: 1 in 20

— Primary Samples: 15 in 20





Major QC Parameters: Blanks

= *An analyte free matrix taken through 'the process' to monitor potential contamination - targeting several key areas*

- Laboratory **Reagent/Instrument** Blanks
- Laboratory **Method** Blanks
- **Field** Blanks
- **Rinsate** Blanks
- **Trip** Blanks





Major QC Parameters: Duplicates (Dups)

= A lab or field split taken through the entire process. This is used to monitor reproducibility or precision

- **Frequency:** 1 in 10 samples

Results are reported & evaluated in Relative Percent Difference (RPD)

$$RPD = \frac{\text{difference between duplicate results}}{\text{average of results}} \times 100$$

- **Lab duplicates** measure the sum of laboratory variation plus sample variation (heterogeneity)
- **Field Duplicates** measure the variation of sampling area



Major QC Parameters: Duplicates (Dups)

= *A lab or field split taken through the entire process. This is used to monitor reproducibility or precision*

- **ALS Acceptance Criteria:**

Both results $< 10 \times \text{LOR}$ $\longrightarrow$ No RPD Criteria

Highest result is $10\text{-}20 \times \text{LOR}$ $\longrightarrow$ RPD $< 50\%$

Highest result is $> 20 \times \text{LOR}$ $\longrightarrow$ RPD $< 20\%$

EXAMPLE:

Standard Pb LOR = 0.001 mg/L

Regular Sample Result = **0.011 mg/L**

Duplicate Sample Result = **0.016 mg/L**

RPD = (Difference/Average) x 100

= (0.005/0.0135) x 100

= 37.04%

CONCLUSION:

RPD must be $\leq 50\%$, duplicate is deemed to pass as the calculated RPD is 37.04%.

Major QC Parameters: Laboratory Control Sample (LCS)

= *A known concentration standard taken through the entire analytical process. It is used to monitor accuracy*

- **Frequency:** 1 in 20 samples
- **Reported in % recovery**

Note that not all compounds will give 100% recovery e.g. some SVOCs



**Low Accuracy
High Precision**



**High Accuracy
Low Precision**



**High Accuracy
High Precision**



Major QC Parameters: Matrix Spike (MS)

= A laboratory split spiked with target analytes prior to sample preparation/analysis. This is used to monitor method interference and accuracy in a given sample matrix.

- **Frequency:** 1 in 20 samples

Results are reported in Percent Recovery (generally between 70-130%)

$$\text{Spike Recovery} = \frac{[\text{Conc. in spiked sample}^* - \text{Conc. in sample}^*] \times 100}{\text{Conc. of spike added}}$$

- **Key Notes:**
 - If sample concentration is >4x spike concentration, results may not be accurate
 - It is best to choose samples which are not highly impacted for MS.
 - Some matrices will not recover spikes.



Major QC Parameters: Surrogates

= *Compounds similar in composition and behaviour to the target analytes but not commonly found in the environment e.g. Toluene with an extra proton added (Deuterated). This is used to measure **sample preparation and analysis plus matrix interference***

- **Key Notes:**
 - Reported in % recovery. Acceptable recovery is generally between 70-130%.
 - Surrogates are only generally used for Organics for 'target analysis' of specific compounds (i.e. not TPH/TRH).
 - High contamination levels may negate ability to report surrogate recoveries



Major QC Parameters: Trip Spikes

= *Laboratory spiked sample sent to the field. These assess losses in transit or due to field practices (e.g. chilling) or even holding times.*

- **Waters:** Spiked with a known concentration samples e.g. 20 µg/L BTEX
- **Soils:** Corresponding Trip Spike Control retained/analysed as additional sample
- **Key Notes:**
 - Analysis cost is charged for both the trip spike and trip spike control
 - Generally only used for BTEXN
 - Must be returned back to issuing laboratory
 - Recoveries are calculated by the consultant

Understanding QC sample requirements



- Whole bottle extractions: SVOCs, PFAS or Oil & Grease in waters



+



+



= Minimum of 2 extra bottle for every 10 primary samples

Primary

Duplicate

Matrix Spike



+



+



= Minimum of 3 extra bottle for every 20 primary samples

Primary

Duplicates

Matrix Spike



QC and QCI Reports

- Completely automated/not subject to human error
- Higher standard than guidelines demand
- Assesses QA/QC parameters
- Highlights QA/QC breaches that might require commentary during reporting.
- Exceptions: They do not assess field QC e.g. field dups or blanks.

QC Report



General Comments

The analytical procedures used by ALS have been developed from established internationally recognised procedures such as those published by the USEPA, APHA, AS and NEPM. In house developed procedures are fully validated and are often at the client request.

Where moisture determination has been performed, results are reported on a dry weight basis.

Where a reported less than (<) result is higher than the LOR, this may be due to primary sample extract/digestate dilution and/or insufficient sample for analysis. Where the LOR of a reported result differs from standard LOR, this may be due to high moisture content, insufficient sample (reduced weight employed) or matrix interference.

Key : Anonymous = Refers to samples which are not specifically part of this work order but formed part of the QC process lot

CAS Number = CAS registry number from database maintained by Chemical Abstracts Services. The Chemical Abstracts Service is a division of the American Chemical Society.

LOR = Limit of reporting

RPD = Relative Percentage Difference

= Indicates failed QC

* = The final LOR has been raised due to dilution or other sample specific cause; adjusted LOR is shown in brackets. The duplicate ranges for Acceptable RPD% are applied to the final LOR where applicable.

Laboratory Duplicate (DUP) Report

The quality control term Laboratory Duplicate refers to a randomly selected intralaboratory split. Laboratory duplicates provide information regarding method precision and sample heterogeneity. The permitted ranges for the Relative Percent Deviation (RPD) of Laboratory Duplicates are specified in ALS Method QWI-EN/38 and are dependent on the magnitude of results in comparison to the level of reporting: Result < 10 times LOR: No Limit; Result between 10 and 20 times LOR: 0% - 50%; Result > 20 times LOR: 0% - 20%.

Sub-Matrix: **WATER**

Sub-Matrix: WATER				Laboratory Duplicate (DUP) Report					
Laboratory sample ID	Sample ID	Method: Compound	CAS Number	LOR	Unit	Original Result	Duplicate Result	RPD (%)	Acceptable RPD (%)
Alk_W: Alkalinity (QC Lot: 7331142)									
NH2601573-003	Test Water 3	Alk_W: Alkalinity	----	1	g CaCO3/m3	20	20	0.0	0% - 20%
Ani_W: Anions by Ion Chromatography (QC Lot: 7331039)									
NH2601573-002	Test Water 2	Ani_W: Sulfate	14808-79-8	0.15	g/m3	1.00	1.00	0.0	No Limit
		Ani_W: Chloride	16887-00-6	0.5	g/m3	1.0	1.0	0.0	No Limit
AT_W: Absorbance/Transmittance by Spectrophotometer (QC Lot: 7331011)									
NH2601573-003	Test Water 3	AT_W: Transmittance	----	0.002	%	0.500	0.500	0.0	0% - 20%
		AT_W: Absorbance	----	0.002	cm-1	0.500	0.500	0.0	0% - 20%
COD_W: Chemical Oxygen Demand (QC Lot: 7331197)									
NH2601573-002	Test Water 2	COD_W: Chemical Oxygen Demand	----	10	g/m3	15	30	66.7	No Limit
DC_W: Dissolved Carbon (QC Lot: 7331217)									
NH2601573-002	Test Water 2	DOC_W: Dissolved Organic Carbon	----	0.5	g/m3	20.0	20.0	0.0	0% - 20%
DO_W: Dissolved Oxygen (QC Lot: 7331209)									
NH2601573-002	Test Water 2	DO_W: Dissolved Oxygen	----	0.1	g/m3	50.0	50.0	0.0	0% - 20%
DRPFIA_W: Dissolved Reactive Phosphorus by Flow Injection Analyser (QC Lot: 7330953)									
NH2601573-002	Test Water 2	DRPFIA_W: Dissolved Reactive Phosphorus as P	----	0.002	g/m3	1.00	1.00	0.0	0% - 20%

QC Report



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Sub-Matrix: WATER				Method Blank (MB) Report	Laboratory Control Spike (LCS) Report			
					Spike Concentration	Spike Recovery (%) LCS	Acceptable Limits (%) Low High	
Method: Compound	CAS Number	LOR	Unit	Result				
PFAS_WSC: Perfluoroalkyl Sulfonamidoethanols (QCLot: 7331401) - continued								
PFAS_WSC: N-Ethyl perfluorooctane sulfonamidoethanol (EtFOSE)	1691-99-2	0.01	µg/L	<0.01	0.01 µg/L	102	80.0	120
PFAS_WSC: N-Methyl perfluorooctane sulfonamidoethanol (MeFOSE)	24448-09-7	0.01	µg/L	<0.01	0.01 µg/L	102	80.0	120
PFAS_WSC: Fluorotelomer Sulfonates (FTS) (QCLot: 7331401)								
PFAS_WSC: 4:2 Fluorotelomer sulfonic acid (4:2 FTS)	757124-72-4	0.01	µg/L	<0.01	0.00937 µg/L	109	80.0	120
PFAS_WSC: 6:2 Fluorotelomer sulfonic acid (6:2 FTS)	27619-97-2	0.05	µg/L	<0.05	0.00951 µg/L	107	80.0	120
PFAS_WSC: 8:2 Fluorotelomer sulfonic acid (8:2 FTS)	39108-34-4	0.01	µg/L	<0.01	0.0096 µg/L	106	80.0	120
PFAS_WSC: Perfluoroalkyl Ether Carboxylic Acids (PFECA) (QCLot: 7331401)								
PFAS_WSC: Hexafluoropropylene oxide dimer acid (HFPO-DA)	13252-13-6	0.01	µg/L	<0.01	0.01 µg/L	102	80.0	120

QCI Report



QA/QC Compliance Assessment to assist with Quality Review

Work Order	: NH2601573	Page	: 1 of 15
Client	: NZ Test Client	Laboratory	: Environmental Hamilton
Contact	: Mr Matt Counsell	Telephone	: +64 7 974 4740
Project	: —	Date Samples Received	: 13-Apr-2026
Site	: —	Issue Date	: 13-Apr-2026
Sampler	: —	No. of samples received	: 5
Order number	: —	No. of samples analysed	: 5

This report is automatically generated by the ALS LIMS through interpretation of the ALS Quality Control Report and several Quality Assurance parameters measured by ALS. This automated reporting highlights any non-conformances, facilitates faster and more accurate data validation and is designed to assist internal expert and external Auditor review. Many components of this report contribute to the overall DQO assessment and reporting for guideline compliance.

Brief method summaries and references are also provided to assist in traceability.

Summary of Outliers

Outliers : Quality Control Samples

This report highlights outliers flagged in the Quality Control (QC) Report.

- NO Duplicate outliers occur.
- Method Blank value outliers exist - please see following pages for full details.
- Laboratory Control outliers exist - please see following pages for full details.
- Matrix Spike outliers exist - please see following pages for full details.
- For all regular sample matrices, where applicable to the methodology, NO surrogate recovery outliers occur.

Outliers : Analysis Holding Time Compliance

- NO Analysis Holding Time Outliers exist.

Outliers : Frequency of Quality Control Samples

- Quality Control Sample Frequency Outliers exist - please see following pages for full details.

QCI Report



Quality Control Parameter Frequency Compliance

The following report summarises the frequency of laboratory QC samples analysed within the analytical lot(s) in which the submitted sample(s) was(were) processed. Actual rate should be greater than or equal to the expected rate. A listing of breaches is provided in the Summary of Outliers.

Matrix: **WATER**

Evaluation: ✖ = Quality Control frequency not within specification ; ✔ = Quality Control frequency within specification.

Quality Control Sample Type		Count		Rate (%)			Quality Control Specification
Analytical Methods	Method	QC	Regular	Actual	Expected	Evaluation	
Laboratory Duplicates (DUP)							
Absorbance/Transmittance in Water	AT_W	1	1	100.00	8.33	✓	ALS New Zealand QC Standard
Alkalinity	Alk_W	1	1	100.00	7.69	✓	ALS New Zealand QC Standard
Anions in Water	Ani_W	1	1	100.00	6.67	✓	ALS New Zealand QC Standard
Chemical Oxygen Demand in Water	COD_W	1	2	50.00	12.50	✓	ALS New Zealand QC Standard
Dissolved Carbon in Water	DOC_W	1	2	50.00	5.26	✓	ALS New Zealand QC Standard
Dissolved Oxygen	DO_W	1	1	100.00	5.26	✓	ALS New Zealand QC Standard
Dissolved Reactive Phosphorus via Flow Injection Analyser	DRPFIA_W	1	1	100.00	8.33	✓	ALS New Zealand QC Standard
Electrical Conductivity in Water	EC_W	1	1	100.00	7.69	✓	ALS New Zealand QC Standard
Fluoride in Water	Fluo_W	1	1	100.00	5.26	✓	ALS New Zealand QC Standard
Heavy Metals Soluble in Water	HMSol_W	1	1	100.00	5.00	✓	ALS New Zealand QC Standard
Heavy Metals Total Recoverable in Water	HMTR_W	1	1	100.00	5.00	✓	ALS New Zealand QC Standard
PFAS in Water (Screen)	PFAS_WSC	0	1	0.00	5.26	✗	ALS New Zealand QC Standard
pH in Water	pH_W	1	1	100.00	7.69	✓	ALS New Zealand QC Standard
Polycyclic Aromatic Hydrocarbons in Water	PAH_W	0	1	0.00	6.67	✗	ALS New Zealand QC Standard
Semi-Volatile Organic Compounds in Water	SVOC_W	1	1	100.00	8.33	✓	ALS New Zealand QC Standard
Semi-Volatile Total Petroleum Hydrocarbons in Water	svTPH_W	0	1	0.00	5.00	✗	ALS New Zealand QC Standard
Total Dissolved Solids in Water	TDS_W	1	1	100.00	10.00	✓	ALS New Zealand QC Standard
Total Kjeldahl Nitrogen as N in Water	TKN_W	1	2	50.00	6.67	✓	ALS New Zealand QC Standard
Total Phosphorus as P in Water	TP_W	1	1	100.00	5.88	✓	ALS New Zealand QC Standard
Total Solids	TS_W	1	1	100.00	10.53	✓	ALS New Zealand QC Standard
Total Suspended Solids	TSS_W	1	1	100.00	11.11	✓	ALS New Zealand QC Standard
Turbidity in Water	Turb_W	1	1	100.00	6.67	✓	ALS New Zealand QC Standard

Laboratory Control Samples (LCS)



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Questions?