

Guidance on Significant Figures for Laboratory Reports

The information below is provided as a guide for the reporting of significant figures for laboratories that undertake analytical procedures in the area of Life Sciences. In particular, the analytical procedures of interest are chemical and biological analyses, but it is applicable to the reporting of most analytical results.

The primary reason that this guidance has been produced is because there is an observed level of difference in the way that laboratories report significant figures. This can create an issue for laboratory clients as they typically compare the analytical results they receive to a standard or guideline value, and whether a result is deemed compliant, or not, to the relevant standard or guideline value can have a range of downstream effects for the client and various regulatory agencies that they may report to.

By detailing a recommended approach to the reporting of significant figures, NATA is seeking to reduce one potential area of variation when an analytical result is compared to a standard or guideline value.

What are significant figures?

The significant figures (which are also known as the significant digits or precision) of a number written in positional notation are those digits that carry meaningful contributions to its measurement resolution. This includes all digits except leading and trailing zeros.”

Measurement resolution is an important phrase here, as the resolution is indicative of the accuracy of the analytical procedure, and can also be used to elude measurement uncertainty or the level of confidence of the analysis at a particular level.

For example, a reported value of 12345 mg/kg would indicate a relatively high degree of accuracy in the area of environmental testing, and could be interpreted (possibly by the untrained client) as meaning that the analytical method that was used to derive this result is capable of differentiating between a concentration of 12345 mg/kg and 12344mg/kg, or 12346 mg/kg. In terms of percentage error, this relates to a 0.0081% difference in the results. As most Environmental Chemists will be well aware, such a low level of analytical error is highly unlikely and, therefore, the advice is to use less significant figures to better reflect the level of confidence in the significant figures presented (for example 12300 mg/kg).

Whilst the piece of analytical equipment used to derive the result of 12345 mg/kg may have presented this as the result, some caution and due diligence needs to be applied to the result to ensure that it accurately reflects the limit of reporting, detection or quantification for the analytical method that was used to derive the result, as well as any limitations with respect to the instrument that was used.

Reference documents

There is some guidance in the literature on the reporting of significant figures; for example, the American Public Health Association's "Standard Methods for the Examination of Water and Wastewater" (widely known as APHA) states:

"To avoid ambiguity in reporting results or in presenting directions for a procedure, it is customary to use "significant figures." All digits in a reported result are expected to be known definitely, except for the last digit, which may be in doubt. Such a number is said to contain only significant figures. If more than a single doubtful digit is reported, the extra digit or digits are not significant. This is an important distinction. Extra digits should be carried in calculation...."

"Report only such figures as are justified by the accuracy of the work."

Therefore, APHA gives an indication of how to report significant figures with the final digit being one that may be in doubt.

American Standard Testing Methods (ASTM) E29-13, section 7.4, provides more clearly defined mechanisms on how many significant figures should be reported. For example, precision based on validation data and/or ongoing QC data (e.g. control charts) could be used to extract standard deviations (sd) at various levels; e.g. at or near the reporting limit (if applicable) and at a more accurate level in the reporting range.

For example from ASTM E29.13 section 7.4:-

Option 1:- The aim is that the rounding interval should not be greater than $0.5 \times \text{sd}$, but not less than $0.05 \times \text{sd}$, the example below may illustrate this better:-

Test result = 123.456, sd = 7.52, hence if the rounding interval is 1, then

$[0.5 \times 7.52 = 3.76] > 1 > [0.05 \times 7.52 = 0.376]$ is acceptable.

Hence one can report the result as 123 (three significant figures) using this rule, as the rounding interval is 1. For a rounding interval of 0.1 (where you would report the result as 123.4 i.e. four significant figures), you have $0.05 \times 7.52 = 0.376$ which is >0.1 and hence is not aligned to this ruling.

Option 2:- There is another option where you look at the sd, if the first digit of the sd is ≥ 2 you would report to the significant figures of that digit, but if the sd is <2 then you'd be able to report a further significant figure e.g.

Test result = 123.456, sd = 2.52, can potentially report 123, as the 1st digit of the sd is ≥ 2 .

Test result = 123.456, sd = 1.52, can potentially report 123.4, as the 1st digit of the sd is <2 .

An example of where too many significant figures are reported is in a recent trace level proficiency program for PFAS in a biota sample, a matrix that is challenging for such analytes given the spike level or entrained level. A laboratory reported the significant figures as below:

Lab Indent.	Result (µg/Kg)	Uncertainty (µg/Kg)	Surrogate Recovery %
XYZ	4.8485	0.8425	216.35

Therefore, based on Option 1, to report a result of 4.8485µg/Kg, the sd for relevant validation data (e.g. replicate fortified matrices near this concentration level) and/or ongoing QC data would need to be <0.02. Expressed as a percentage, $0.02/4.8485 = 0.412\%$ relative standard deviation (%RSD). Such precision for trace level PFAS analysis in a validation is highly unlikely, and in routine QC data even less likely. Hence, the use a lower number of significant figures is justified and should have been used. Typically, the Uncertainty reported should have less significant figures than the reported Result, as there is a significant error associated with Uncertainty determinations.

In the opinions of the authors, in this specific case, the result should be rounded to two significant figures i.e. 4.8 µg/Kg to reflect the resolution of the analytical procedure in this circumstance. There are always some professional and defensible judgements that can be applied, but a conservative approach is recommended in order to avoid misleading the client and the level of confidence in the reported values!

Another document that provides advice on significant figures is the Australian Drinking Water Guidelines (ADWG), in its section on guidance on the rounding of results.

This section states that the:

The vast majority of numerical guideline values in the ADWG are rounded to a single significant figure. Consistent with standard rounding convention, mid-way values are rounded up. For example, 1.5 is rounded to 2 and 25 is rounded to 30. Trailing zeros in numbers where there is no decimal point should not be taken as significant (e.g., nitrate, 50 mg/L).

Practically all of the health-based guideline values were established using data and assumptions with a precision of one significant figure (e.g., volume of water consumed by an adult = 2 L/day). Furthermore, the vast majority include the incorporation of safety factors, which are applied at the precision of 'order of magnitude' (e.g., 10 for interspecies extrapolation and 10 for intra-species variation).

Quoting more significant figures misrepresents the degree of calculated precision and may lead to unfounded concern when guidelines are exceeded at the second or third significant figure.

It is noted that exceptions to this may be necessary for some chemicals. These will be considered on a case-by-case basis and the reasons for the deviation from the convention of rounding to a single significant figure will be explained in the [related] fact sheet.

It is noted that aesthetic guidelines are generally based on direct information on palatability to consumers, including appearance, taste and odour, and so do not need to be rounded.

Recommended approach to significant figures

In the first instance, the number of significant figures that are quoted in an analytical result should reflect the accuracy of the analytical technique used to derive the result.

If in doubt as to how many significant figures should be quoted in an analytical result, apply the significant rules described in ASTM E29-13.

In consultation with the client, or relevant regulatory agency, and where it is justified to do so, if the analytical result is going to be compared to a standard or guideline value in order to determine compliance with the standard or guideline value, the analytical result should contain the same number of significant figures as standard or guideline value, or no more than one additional significant figure.