Rounding and Significant Figures

Laboratory Analytical Procedure (LAP)

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Procedure Title: Rounding and Significant Figures

Laboratory Analytical Procedure

1. Introduction
   1.1  This procedure describes the rules for rounding numbers for the reporting of analytical data.

2. Scope
   2.1  This method describes the application of significant figures for the proper reporting of analytical data.

3. Terminology
   3.1  Significant Figures: The number of significant figures in a measured quantity is the number of digits that are known accurately, plus one that is in doubt. Zeros that appear to the left of the first nonzero digit are placeholders and are not considered significant. Zeros located to the right of the first digit may be considered significant.
   3.2  Analytical Data: Data that represent the measured concentration or value of analytes in a sample aliquot. Sample aliquots include samples, method blanks, calibration verification standard (CVS) and quality assurance samples (QA samples, e.g. NIST standards).
   3.3  Sample Data: Data that represents the measured concentration of analytes in a sample.
   3.4  Method Blank Data: Data that represent the measured concentration of analytes measured in all reagents without the addition of a sample.
   3.5  Quality control (QC) Data: Data that represent the measured concentration of target analytes that are elements of QA and CVS samples.
   3.6  Quality Assurance Data: Data that represent the known values in a standard reference material.
   3.7  Accuracy Data: Data that represent the percent recovery determined from QC data.
   3.8  Precision Data: Data that represent the relative percent difference or relative standard deviation calculated from accuracy data.
   3.9  Calibration Range: The range of a method is defined as the lower and upper concentrations for which the analytical method has adequate accuracy, precision and linearity.

4. Significance and Use
   4.1  It is the responsibility of each analyst recording analytical data to comply with each of these rules for significant figures and rounding.
   4.2  It is the responsibility of each supervisor, data reviewer, or QA representative to ensure that these rules are properly applied in the treatment of analytical data.

5. Interferences
   5.1  Not applicable
6. **Apparatus**

   6.1 Not applicable

7. **Reagents and materials**

   7.1 Not applicable

8. **ES&H Considerations and Hazards**

   8.1 Not applicable

9. **Procedure**

   9.1 All calculations should be completed prior to any rounding to avoid introducing additional error into the analytical result.

   9.2 Data entry into calculators or computers should include all of the available digits from the analytical instrument generating the data. Some instrument outputs contain an excessive number of digits. In these cases, data entry should be at least 5 digits (if available) to prevent error due to successive rounding.

   9.3 The calibration range must be reported using the same rounding and significant figures rules as the associated sample data.

   9.4 Data below the calibration range prior to rounding should be reported as <(the lower end of the calibration range). Example: If your calibration range is 500 - 100 ppm, and your instrument reports a value below 100 ppm, the data should be reported as “<100 ppm”.

   9.5 Results from the measurement of Method Blank samples results should be treated as analytical data and reported with the same number of significant figures as the associated sample data.

10. **Rounding Rules**

   10.1 When the digit following the last significant digit is less than 5, the number remains unchanged (round down.)

       *Example:* 1.63 is rounded to 1.6

   10.2 When the digit following the last significant digit is greater than 5, the digit to be retained is increased by 1.

       *Example:* 2.6 is rounded to 2.7

   10.3 When the digit following the last significant digit equals 5, the number is rounded off to the nearest even number.

       *Example:* 3.85 is rounded to 3.8, 4.55 is rounded to 4.6

   Note: Some automated systems such as spreadsheets, calculators and data management software always round up a five.

   10.4 When calculations are complete and two or more figures are to the right of the last the last significant digit, rounding begins at the least certain digit and continues until the correct number of digits remains.

       *Example:* Rounding to two significant figures:

       2.4501 is viewed as 2.4(501) and is rounded to 2.5

       2.5499 is viewed as 2.5(499) and is rounded to 2.5
10.1 Significant Figures

10.1.1 The rounding rules described in Section 10 must be used to report data to the proper number of significant figures. This section describes how to determine the proper number of significant figures.

10.1.2 The number of significant figures in a measured quantity is the number of digits that are known accurately, plus one that is in doubt. Zeros that appear to the left of the first nonzero digit are placeholders and are not considered significant. Zeros located to the right of the first digit may be considered significant. The concept of significant digits applies only to measured quantities and to results calculated from measured quantities. It is never applied to exact numbers or definitions.

Example: 15.8 sec ÷ 60 sec/min = 0.263 min the answer has three significant figures because the conversion factor is a definition.

10.1.3 A final result should never contain any more significant digits than the least precise data used to calculate it.

11. Calculations

11.1 To report or calculate the relative percent difference (RPD) between two samples, use the following calculation

\[ RPD = \left( \frac{X_1 - X_2}{X_{\text{mean}}} \right) \times 100 \]

Where:

- \( X_1 \) and \( X_2 \) = measured values
- \( X_{\text{mean}} \) = the mean of \( X_1 \) and \( X_2 \)

11.2 To report or calculate the root mean square deviation (RMS deviation) or the standard deviation (std. dev.) of the samples, use the following calculations.

First find the root mean square (RMS), of the sample using

\[ RMS = x_m = \text{mean} = \sqrt{\frac{\sum_{i=1}^{n} x_i}{n}} \]

Then find the root mean square deviation, or standard deviation, using

\[ RMS_{\text{deviation}} = \sigma = \text{stddev} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - x_m)^2}{n}} \]
Where:

\[ x_m = \text{the root mean square of all } x \text{ values in the set} \]
\[ n = \text{number of samples in set} \]
\[ x_i = \text{a measured value from the set} \]

12. **Report Format**
   12.1 Not applicable

13. **Precision and Bias**
   13.1 Not applicable

14. **Quality Control**
   14.1 Not applicable

15. **Appendices**
   15.1 Not applicable

16. **References**