STATISTICS IN CHEMISTRY

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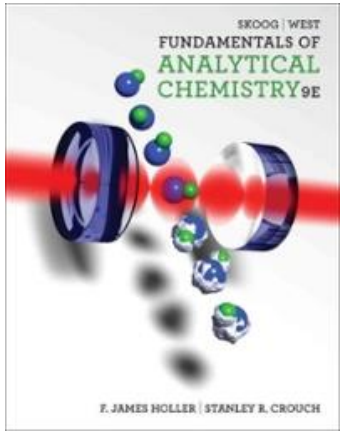

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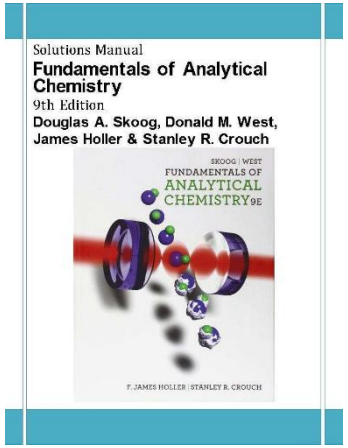


1. Skoog DA, West DM, Holler FJ, Crouch SR. Fundamentals of Analytical Chemistry. Nelson Education; 2013.
2. Skoog DA, West DM, Holler FJ, Crouch SR. Solutions Manual of Fundamentals of Analytical Chemistry. Nelson Education; 2013.

Sampling, Standardization and Calibration

Sampling

Sampling is one of the most important steps in an analytical process. The sample should represent the population on which you want to be informed. Unless the analyzes are performed on the representative sample, no matter how high and precise the analysis is, they make no sense.

Analyses can be classified according to the sample size used in the analysis; macro, semi-micro, micro and ultra micro analysis.

Analyses are also classified as major constituent analysis, minor constituent analysis, trace constituent analysis and ultra trace constituent analysis according to the constituent types.

The sampling steps can be summarized as follows:

* *Raw sample*: The first sample taken to represent the population. The sample size varies depending on the heterogeneity of the sample and the size of the beads in the sample. The higher the particle size and heterogeneity, the larger the sample size.

* *Laboratory sample*: The raw sample is the sample taken after grinding by reducing the particle size and blending the whole batch thoroughly to be sent to the laboratory for analysis. 3 samples are taken from the laboratory sample. One of them is sent to the laboratory for analysis, one remains with the customer, and one is maintained for use as a witness sample in case of any dispute.

* *Analysis sample*: This is the sample taken as a representative sample from the mixture after grinding and blending the sample to the laboratory into smaller particles.

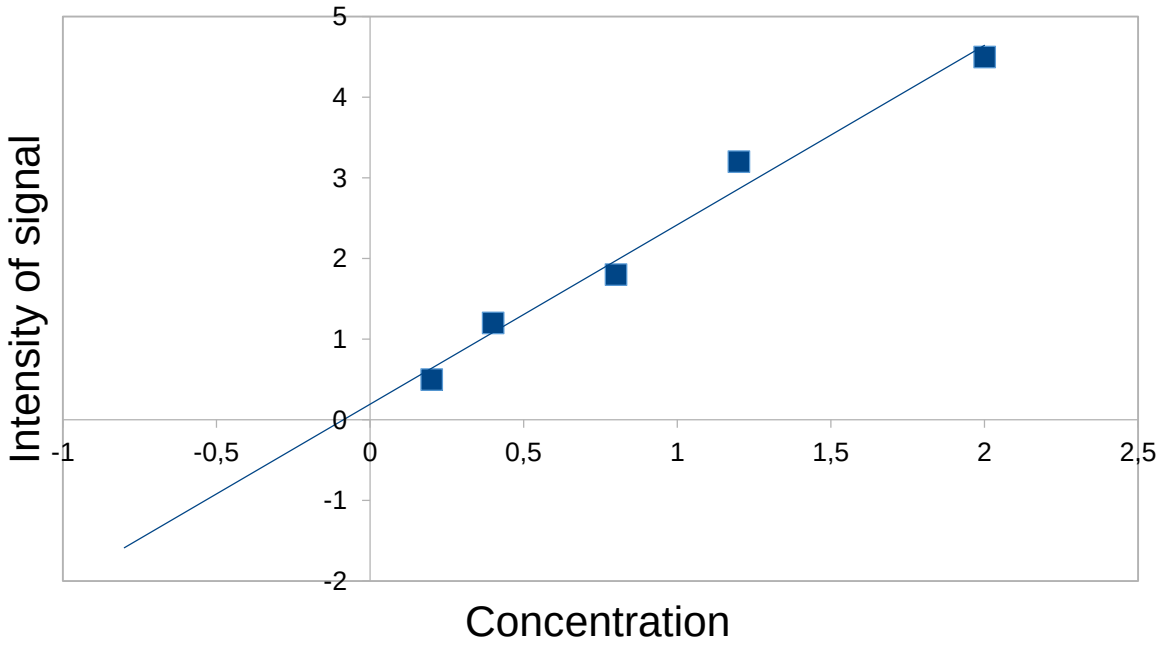
* *Test sample*: It is the portion of the sample that is taken from the analysis sample by weighing or otherwise measured and on which the analysis is performed.

Standardization and Calibration

Calibration is the process of determining the relationship between analyte concentration and an analytical signal. Here the signal can be any physical property that can be measured by color intensity, current, potential, pH, resistance, etc. There are different procedures applied for this purpose.

One of them is the comparison process with standards. In this process, the signal intensity of the sample is directly compared with the signal intensity of a substance used for reference to obtain information about the concentration of analyte in the sample.

Another procedure is the calibration with the external standard. In this process, a series of standard solutions of different concentrations are prepared from a standard substance of the analyte to be determined, separate from the sample, and the intensity of the signals obtained by the analytical method is measured on these standard solutions. The signal intensity against the known concentrations of standard solutions is plotted on a graph. The resulting graph is called the calibration graph. The difference between the experimental points in the calibration graph and the point at which the vertical line drawn from this point to the x axis intersects the calibration graph is called the experimental error.



The signal intensity of the analyte in the test sample is measured by the same method as for the calibration solutions. This signal intensity is marked on the y-axis in the calibration graph and drawn in a line parallel to the x-axis. A straight line is drawn from the point where this line intersects the calibration line and the analyte concentration is read from the point where the line intersects the axis.

Finding mathematical model of calibration graph - Least squares method

The mathematical model of the calibration graph is also called the regression model. The least squares method used in the calculation of this model assumes that the measured signal intensity is directly proportional to the concentration, and that the deviation at each measured point results from the measurement error only.

In the application of the least squares method, manual calculations can be performed, as well as various computer programs can be used to facilitate the calculations.

In order to reduce errors due to differences in the matrix of the sample and calibration solutions in the external calibration processes, the raw signals obtained from the measurements are corrected using blank signals. As the blank, the ideal blank can be used or, as this is often not possible, the solvent blankor reactive blank can be used instead of the ideal blank.