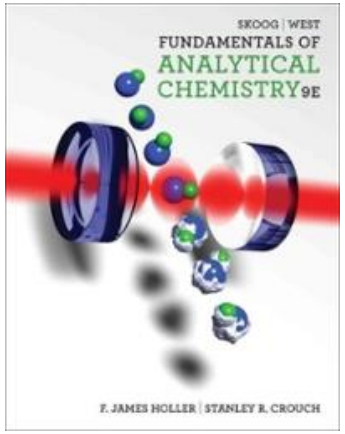
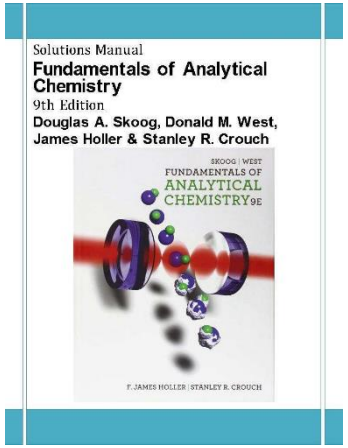
STATISTICS IN CHEMISTRY

1.



2.



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.

Calibration, Sensitivity, Detection Limit, Control Cards, Validation

Calibration

Calibration is the process of finding the relationship between analyte concentration and analyte-related measured signal. Almost all methods used in the measurements require a calibration process using chemical standards. Calibration is performed using linearity or conversion to linearity of the relationship between the measured physical magnitude (absorption, conductivity, potential, current intensity, peak area, etc.) against the known analyte concentration. However, calibration may not be necessary for some analytical methods such as coulometric methods, gravimetry, titrimetry.

In the ***internal standard method***, the sample is made by adding solutions containing known amounts of reference species to the standards to the blank solution. Instead of using the analyte signal, the ratio of the reference species to the analyte signal is used.

If there is no interfering species in the sample components, external standards are used. The external standard is a series of solutions containing known concentrations of analyte prepared separately from the sample.

Calibration Sensitivity and Limit of Observation

Calibration sensitivity: It is the ratio of the change in the amount of the unit to the change in the signal intensity. Briefly the slope of the calibration graph.

Analytical sensitivity: The ratio of the slope of the calibration graph to the standard deviation of the signal intensity of the analyte (sometimes used as blank test solutions) for a constant concentration.

Detection limit: All methods applicable to analyte determination have an detection limit. It is the lowest concentration that can be determined by applying that method. The slope, m, of the calibration graph is calculated from the following equation by taking the standard deviation, sb, of the signals read from the blank test solution and a coefficient k or 3k used for a given confidence level:

$$DL = \frac{k \; x \; s_b}{m}$$

Linear Dynamic Range: This is the range that can be determined by the calibration graph. The lowest concentration value of this range is considered the limit of detection. The upper limit is expressed as the concentration at which the calibration graph deviates from linearity by 5%.

Control cards: Graphs of changes in concentration generated over time. These graphs have lower control limit and upper control limits, which means no problem when the values obtained are within this range. When it goes beyond these limits, it is considered an error indicator.

$$\text{UCL} = \mu + \frac{3\sigma}{\sqrt{N}}$$

$$\text{LCL} = \mu - \frac{3\sigma}{\sqrt{N}}$$

Validation: It is the process of determining whether the analysis is at the desired level. Confirmation is used for verification purposes.