Glossary of Analytical Terms

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by

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Abstract

The following glossary defines the most common terms encountered in analytical chemistry. Many of these terms are used interchangeably in common usage. Describing chemical measurement procedures and results requires that we use accepted terminology to avoid confusion. For most terms I follow recommendations by IUPAC and note any deviations.[1] Other fields of science and engineering might have slightly different conventions, so use the context to eliminate any ambiguity.

The current version of this document is available online at:

http://www.files.chem.vt.edu/chem-ed/a-text/.

For use with B. M. Tissue, *Basics of Analytical Chemistry and Chemical Equilibria* (John Wiley: New York, 2011).

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[1] *IUPAC Compendium of Chemical Terminology - the Gold Book* (International Union of Pure and Applied Chemistry: Research Triangle Park, NC, 2005-2009); available: http://goldbook.iupac.org/index.html, Release 2.1.5, 2009-09-07.

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A – C

accuracy

The closeness of an experimental measurement to the true value.

analyte

The chemical species to be identified or quantitated. Can be a pure substance or one constituent of a multi-component sample.

baseline

The average value of blank measurements. For spectral and chromatographic data, the average minimum where there are no peaks. For spectra it might also refer to the average value of a reference spectrum.

bias

see *error, systematic*

blank

A standard that contains no analyte, i.e., a concentration of 0.0. The composition should otherwise match the sample solution. Variations include method, equipment, and instrument blanks for blanks that go through all or only part of the sample processing procedures.

blank, field

A blank prepared in the field that goes through all sample processing and analysis procedures. A variation is a spiked field blank.

calibration

The process of measuring a known quantity to determine the relationship between the measurement signal and the analyte amount or concentration.

calibration curve

A plot of signal versus analyte amount or concentration for multiple standards. Used to calibrate a measurement over an extended range.

calibration function

The mathematical equation that is the best fit to the data in a calibration curve.

contaminant

A substance, including the analyte itself, that is introduced unintentionally into a sample during collection, processing, or measurement.

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C – E

control chart

A plot versus time of the results of one or more control samples. Usually includes the upper and lower limits to specify if a method or instrument is within or out of control.

control samples (quality control samples)

The blanks, standards, and spiked samples that are measured to determine the accuracy of a measurement.

duplicate sample

A sample that is split into two portions to monitor method variability. A method will often specify analysis of duplicate samples at some frequency based on time or number of collected samples. See also *replicate measurements*.

false positive

Determination that an analyte is present in a sample that had no analyte. Causes include contamination or memory effects.

false negative

Inability to detect an analyte that is present above the detection limit. Occurs due to analyte loss in sample processing or interferences obscuring the true signal.

drift

The gradual change in blank measurements over time.

qualitative analysis

Making measurements to determine the identity, structure, or physical properties of a substance.

quantitative analysis

Making measurements to determine the amount of an analyte in a sample.

detector

A device that responds to the presence of analyte, usually generating an electrical output.

dynamic range

The ratio of the maximum to the minimum measurable signal. The maximum is determined by the point at which the signal no longer increases with increasing analyte concentration and the minimum is chosen as the LOD. See also *linear range*.

error, random

The spread in replicate measurements due to random fluctuations.

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E – M

error, systematic

The difference between a measurement and the true value.

good laboratory practice (GLP)

Specific regulations in the Code of Federal Regulations by which laboratories must conduct, verify, and maintain their procedures, results, and records.

interference

A component that is in or is introduced into a sample that causes a measurement to be higher or lower than the true value.

IUPAC (International Union of Pure and Applied Chemistry)

A non-governmental agency that recommends standardization of chemical nomenclature, terminology, and chemical and physical data.

limit of detection (LOD)

The minimum concentration at which an analyte can be reported as detected. Determined from a signal level that is 3 times the baseline noise.

limit of quantitation (LOQ)

The minimum concentration at which an analyte concentration can be reported. Determined from a signal level that is 10 times the baseline noise.

linear range

of an analytical method or instrument is the range of concentrations that fall in the linear range.

linear regression

A calculational method using least squares to determine the best linear equation to describe a set of x and y data pairs.

matrix effects

Systematic errors due to details of the sample matrix.

memory effect

An apparent signal from an instrument that occurs due to contamination from a previous sample.

method development

Determining the experimental conditions for sample collection, preparation, and measurement that produce accurate and repeatable results.

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M – R

method validation

Performing control experiments to verify the *accuracy, sensitivity, specificity, and reproducibility of test methods*. [Italized terms from 21 CFR 211.165 (e).]

noise

Random fluctuations in the signal. Usually quantified using the standard deviation of multiple measurements of a blank.

precision

The repeatability in making replicate measurements. Imprecision, or the lack of precision, is probably a better term to describe the repeatability of measurements, but precision is the more common term. Quantitative measures include standard deviation, standard error, and confidence limits.

quality assurance

Auditing of methods and procedure to ensure accurate results.

quality control

Procedures of instrument calibration and method validation to produce accurate results.

repeatability

Comparison of replicate measurements made on the same sample and performed under identical conditions.

replicate measurements

Multiple measurements of the same sample. Replicate measurements are made by dividing the sample into several portions and measuring each portion separately. Doing replicate measurements provide a measure of precision of the method and can identify outliers due to gross errors such as omitting one step in a procedure, one-time instrument glitches, or recording a value incorrectly.

reproducibility

Comparison of replicate measurements made on the same sample by different analysts or different methods. The calculations of precision are the same for repeatability and reproducibility, the difference is the source of the measurements being described.

robustness

The impact that variable experimental conditions, such as temperature, pH, ionic strength, etc, can have on a measurement.

ruggedness

See *reproducibility*.

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S – S

selectivity

The discrimination of an analyte versus other components in the sample.

sensitivity

The proportionality factor of the measurement, i.e., slope of the calibration function.

sensitivity

The change in detector signal versus change in analyte concentration.

signal

The detector output that is displayed or recorded.

signal-to-noise ratio (S/N or SNR)

The ratio of the signal to the baseline noise.

signal averaging

Recording and averaging a signal for some number of measurements or for some time period to improve the signal-to-noise ratio. The sample is not changed, which distinguishes signal averaging from making replicate measurements.

smoothing

Averaging adjacent points in a spectrum or plot to reduce the noise.

specificity

The ability of a method or instrument to measure an analyte in the presence of other sample components.

spike

An internal standard or standard addition added to a sample or blank.

stability

Retention of analyte over time or during sample preparation and analysis steps.

standard

A sample of known composition prepared from a certified reference material.

standard, internal

a standard that is added directly to the sample. The internal standard is then measured simultaneously with the analyte.

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S – Z

standard, primary

a reagent that is extremely pure, stable, has no waters of hydration, and has a high formula weight.

standard, secondary

a standard that is prepared in the laboratory or by a third party for a specific analysis. It is usually standardized against a primary standard.

standard-addition method

involves adding a known amount of the analyte, a spike, to the sample to provide an ``internal'' calibration to the measurement.

standard operating procedure (SOP)

A document containing the instructions for a specific analytical procedure or instrument

trace analysis

Measurement of analyte concentrations of less than approximately 100 ppm.

validation

See *method validation*.

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