Abstract
The following glossary defines common terms encountered in analytical chemistry. Many of these terms are used interchangeably in day-to-day language. Describing chemical measurement procedures and results requires the use of accepted terminology to avoid confusion. I follow IUPAC recommendations for most terms, noting any deviations. See references 1 and 2 for general terminology. Other fields of science and engineering might have slightly different conventions, so use the context to eliminate ambiguity. As an example, speciation has very different meanings between chemists and biologists.

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A – B

accuracy
The nearness of an experimental measurement to the true value. For test portions containing unknown amounts of analytes, the accuracy of a given method is inferred from the accuracy when measuring certified reference materials.

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

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

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

background
The detector signal for a physical measurement, concentration, spectrum, or chromatogram when no test portion is present. May also refer to the normal or unperturbed concentrations in biological or environmental samples.

baseline
Synonymous with background, but usually in reference to data plotted in a spectrum or chromatogram. The average value of blank measurements. For spectral and chromatographic data, the average minimum where there are no peaks. When the baseline is sloped, the baseline value for a given peak can be interpolated from the edges of the peak.

bias
See error, systematic.

blank
A standard that contains no analyte, i.e., a concentration of 0.0. The composition, solvent, electrolyte, etc, should otherwise match the sample test portion. 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. The field blank is useful to monitor for sample contamination. A variation is a spiked field blank to monitor loss of analyte due to sample processing, etc.
**C – D**

**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. Used to calibrate a measurement over an extended range. Good practice is to measure five to ten standards that are equally spaced through the measurement range.

**calibration function**
The mathematical equation that is the best fit to the data for a set of calibration data.

**carry over**
Residual analyte in a sample preparation or measurement step that causes a measurement to be higher than the true value. See memory effect.

**certified reference material (CRM)**
A material that is verified to contain a known amount of analyte(s) or to have known physical properties. Usually available from commercial suppliers. Also referred to simply as reference material (RM). See [http://nist.gov/srm/definitions.cfm](http://nist.gov/srm/definitions.cfm) for more details.

**contaminant**
A substance, which can include the analyte itself, that is introduced unintentionally into a sample or test portion during collection, processing, or measurement.

**control chart**
A plot versus time of measurement 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 test portions that are measured to determine the accuracy of a measurement.

**dark current or dark signal**
The detector output when the detector is shielded from any input.

**dark spectrum**
The dark signal as a function of wavelength or energy. Measured and stored (with a reference spectrum if measuring absorbance) in array-detector spectrometers to calculate the spectrum of the test portion.
**detection limit**
See *limit of detection or method detection limit*.

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

**difference spectrum**
A spectrum obtained by subtracting a reference spectrum from a measured spectrum to show changes between the two spectra. Peaks can be positive or negative.

**drift**
The gradual change in blank measurements over time.

**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*.

**dynamic range**
The ratio of the maximum to the minimum measurable analyte concentration. The maximum is determined by the point at which the signal no longer increases with increasing analyte concentration. The minimum is chosen as the limit of detection (LOD). For linear dynamic range, the maximum is the point at which the signal deviates from linearity. See also *range*, *measurement*.

**E – L**

**EPA action level**
The concentration of a contaminant that requires a response such as public notification, exposure monitoring, or remediation.

**error, random**
The spread in replicate measurements due to random fluctuations. Will be both higher and lower than the true value.

**error, systematic**
A consistent difference either higher or lower between an experimental measurement and the true value. Can differ from sample to sample depending on variability in sample matrix effects.

**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.

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 or test portion that causes a measurement to be higher or lower than the true value. Often due to overlap of peaks or chemical conversion of analyte to a different form. The term usually refers to a specific species rather than systematic errors caused by the summation of matrix effects.

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 measured concentration at which an analyte may be reported as being detected in the test portion or sample. There are several accepted methods to determine an LOD. A simple method is to calculate the concentration that corresponds to a signal level that equals the baseline plus 3 times the noise. See also method detection limit.

limit of linearity (LOL)
The concentration at which the signal deviates from linearity.

limit of quantitation (LOQ)
The minimum measured concentration at which an analyte concentration may be reported. A simple method is to calculate the concentration that corresponds to a signal level that equals the baseline plus 10 times the noise.

linear range
See range of linearity.

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

**masking reagent**
A reagent added to a test portion to prevent sample components from interfering in an analytical method. An example is the chelating ligand in total ionic strength adjustment buffer (TISAB) that is used with a fluoride ion selective electrode (ISE). The ligand prevents metal ions such as Fe$^{3+}$ and Al$^{3+}$ from forming fluoride complexes.

**matrix effect**
The effect on a measurement resulting from components in the sample. Can vary sample to sample and impact the result higher or lower. Specific species that are identified as causing a systematic error are called interferences.

**memory effect**
An apparent signal in an instrumental measurement that occurs due to contamination or carryover from a previous test portion.

**method detection limit (MDL)**
...the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero and is determined from analysis of a sample in a given matrix containing the analyte. [Italicized terms from 40 CFR 136 Appendix B.] See also reference.5

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

**method validation**
Performing control experiments to verify the accuracy, sensitivity, specificity, and reproducibility of test methods. [Italicized 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.
**protecting reagent**
A reagent added to a test portion to prevent the analyte(s) from being lost or otherwise not detected. An example is a weak complexing agent to prevent metal ions from precipitating as insoluble hydroxides at high pH.

**qualitative and quantitative analysis**
See analysis, qualitative and analysis, quantitative.

**quality assurance**
Auditing of methods and procedures to ensure accurate results.

**quality control**
A system of instrument calibration and method validation procedures to produce accurate results.

**R**

**range of linearity**
The range of concentrations for which the signal responds linearly to analyte concentration. The lower limit may be taken as zero and the upper limit is where the signal versus concentration deviates from linearity.

**range, measurement**
The range from the minimum to the maximum measurable analyte concentrations. The minimum may be taken as zero or chosen as the limit of detection (LOD). The maximum is determined by the point at which the signal no longer increases with increasing analyte concentration. For linear dynamic range, the maximum is the point at which the signal deviates from linearity. Not to be confused with dynamic range, which is a ratio.

**reference spectrum (for instrument operation)**
The spectrum of a pure solvent or reference substance. Measured and stored in array-detector spectrophotometers to calculate the absorption or reflectance spectra of test portions. Also used to convert measured spectra to difference spectra.

**reference spectrum (of a material)**
The spectrum of a certified reference spectrum. Useful for comparison to identify or determine the purity of test portions.

**repeatability**
Comparison of replicate measurements made on the same sample or test portion and performed under identical conditions. The typical descriptor is the standard deviation of the measurements.
replicate measurements
Multiple measurements of the same laboratory sample. Replicate measurements are made by dividing the sample into several test 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 (blunders) 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 test sample by different analysts in different laboratories. The calculation of precision is the same for repeatability and reproducibility, the difference is the source of the measurement results.

resolution
The minimum difference between separated peaks in a chromatogram or spectrum. Specific definitions can be found for chromatograms and mass spectra.

resolution, spectrometer
The minimum bandpass of a spectrometer.

resolving power
A measure of resolution, usually $m/\Delta m$ in mass spectrometry. The criteria for separated peaks must be specified for determining $\Delta m$.

response factor or relative detector response factor ($f$)
The relative sensitivity of a detector for an analyte and a standard. May be less or greater than 1.0. Most commonly used in chromatography with an internal standard.

robustness
See ruggedness.

ruggedness
The degree to which variable experimental conditions, such as temperature, pH, ionic strength, etc, will affect the accuracy and precision of a measurement result. See also reproducibility.

S

sample
A portion of material selected from a larger quantity of material. [Italicized terms from IUPAC Gold Book.]

sample, laboratory
A sample as delivered to the testing laboratory.
**sample, test**
A sample that has been processed in the laboratory and is ready to divide into test portions.

**sampling plan**
The method by which samples are collected from a population. Common selection methods use random, systematic, or stratified strategies.

**selectivity**
The ability of a method or instrument to measure an analyte in the presence of other constituents of the sample or test portion.


**sensitivity**
The slope of the calibration function, i.e., the change in detector signal versus the change in amount of analyte. For non-linear calibration functions, the sensitivity will be a function of concentration. Not to be confused with limit of detection. A higher sensitivity may allow measurement of a lower analyte concentration, depending on the signal-to-noise ratio.

**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 period of time to improve the signal-to-noise ratio. The test portion is not changed, which distinguishes signal averaging from making replicate measurements.

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

**speciation analysis**
The determination of the specific forms of an analyte. Common examples are elemental mercury versus organomercury and different oxidation states such as Cr(III) versus Cr(VI).

**species, chemical**
A specific form of an atomic or molecular entity.

**specificity**
See selectivity.
**spectrum**
A plot of signal versus wavelength or energy.

**spike**
An internal standard or standard addition added to a test portion or blank.

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

**standard**
A sample or test portion of known composition prepared from a certified reference material.

**standard, internal**
A standard that is added directly to the test portion. The internal standard is then measured simultaneously with the analyte.

**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**
A calibration method of 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.

**T – Z**

**test portion**
A portion of a sample that is tested or analyzed.

**trace analysis**
Measurement of analyte concentrations of less than approximately 100 ppm.
**ultra-trace analysis**
A term with no standard definition. Typically used for measurement of analyte concentrations of less than approximately 1 ppb or less.

**unknown**
A term with no standard definition. The source of the sample is usually known. Calling a sample an “unknown” is common usage to indicate that the analyte concentration in the sample is unknown.

**validation**
See *method validation*.

**References**