Glossary of Terms

Metadata

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Term	Definition
Absolute technique	Analytical technique involving a chemical reaction which achieves stoichiometric completion in accordance with the chemical equation fro that reaction
Absorptivity	A constant term which reflects the ability of the analyte to absorb radiation at a particular frequency
Abundance	Abundance in this context refers to the quantity of a solid present within another solid matrix. (Note: within a liquid matrix, the term used would be concentration
Acceptable bias	A value for bias considered small when compared to the method's precision
Acceptance criteria	The set of analytical values that a product must achieve in order for it to meet the agreed product specification.
Accreditation	The procedure by which an authoritative body gives formal recognition that a body or person is competent to carry out specific tasks
Accredited laboratories	Laboratories that have submitted themselves to an approved system of accreditation and have satisfied all of the necessary requirements (see accreditation)
Accuracy	The closeness of agreement of a test result and the accepted reference value
Active sampling	A form of continuous sampling whereby the sample is drawn by a pump over or through a chemical reagent or adsorbent. (see continuous sampling)
Activity	The effective concentration of an ion in the presence of an electrolyte. It is defined mathematically as activity = concentration X activity coefficient. At very low concentrations (less than 10^{-4} M) the value of the activity coefficient approaches 1 and thus activity = concentration. At higher concentrations, the value of the activity coefficent is less that 1 and thus activity becomes less than the apparent concentration.
Adjusted retention time (volume)	The time that it takes for an analyte to elute from a chromatographic column after injection, minus the time it takes for an unretained analyte to elute from the column under the same experimental conditions
Amperometry	Amperometry is the application of voltammetric measurements at a fixed potential to detect changes in current flow as a function of concentration - see voltammetry

Anode	The electrode in an electrolytic cell where oxidation occurs
Anti-Stokes lines	Scattered photons that have a lower wavelength (higher energy) than the incident light.
Audit	A systematic independent and documented process for evaluating if specific quality requirements have been fulfilled
Beer's law	The absorbance(A) = -log transmittance (T) = absorptivity (a) X pathlength (b) X concentration (c)
Bias	The difference of the mean value of a set of measurements and the reference value
Bioluminescence	The emission of visible radiation from living systems as a result of enzyme catalysis
Blank	See 'blank signal'
Blank signal	The measurement made on a calibration sample, following an established procedure, but where the analyte has not been deliberately added.
Blind samples	A sample of known characteristics which is presented for analysis as a genuine sample. It is used to monitor the performance of individual analysts or methods
Calibration function	The term in the equation that relates the instrument signal to analyte concentration. This term is constant over the range where there is a linear relationship
Capacity factor	A relative mathematical term given the symbol (k' or k) used in high performance liquid chromatography for the reporting of qualitative data
Capillary electrophoresis	The transport of electrically charged compounds in solution under the influence of an electric field
Capillary gas chromatographic column	A length of silica glass tubing (0.1-0.5 mm internal diameter and 10-100 m in length) with an external coating of a polyimide. The inside of the capillary is coated with 0.1-1.0 µm of a liquid stationary phase
Carrier gas	The inert gas used to transport solutes through a gas chromatographic column from the point of injection to detection

Cathode	The electrode in an electrolytic cell where reduction occurs
Certified reference material	A reference material where one or more properties of the material have been certified by a technically valid procedure. It is accompanied by or traceable to documentation issued by the certifying body
Chemical ionisation mass spectromery	A lower energy form of mass spectrometry whereby excitation of the analyte molecule occurs following collision with energetic ions created within the mass spectrometer
Chemiluminescence	A process whereby the products of a chemical reaction emit radiation in the visible region of the electromagnetic spectrum
Chemometrics	The application of mathematical or statistical methods to chemical data..
Chromatogram	A graphical representation of the analytes separated on a chromatographic column
Chromatograph	A sophisticated instrument used to separate analytes through the process of chromatography
Chromophore	Groups within a molecule that give rise to absorption bands in definite regions of the UV/visible regions of the electromagnetic spectrum.
Coagulation	The process whereby non-settleable colloidal residues are destabilized by the addition of aluminium salts with rapid mixing, resulting in the formation of settleable flocs.
Column packing	A support material of high surface area which has been coated with a thin layer of a liquid stationary phase.
Combination bands	Bands in the IR spectrum brought about by the combination of the fundamental symmetric and asymmetric stretching vibrations. These combination bands are normally found in the near infrared region of the electromagnetic spectrum.
Comminution	The general term used to describe processes for particle size reduction and includes crushing, grinding, pulverising etc.
Comparative technique	An analytical technique which required calibration against known standards in order for accurate analytical data to be obtained

Composite sample	The combination of increments, each taken from a sampling unit related to a single consignment (see consignment)
Concentration polarisation	The condition in an electrochemical cell where the transport of of species to and from an electrode surface is insufficient to maintain the current at a desired level
Consignment	A sampling entity (batch) that is likely to comprise a number of individual sampling units. For instance a batch stored in a warehouse, comprising a number of individual boxes, each of which represented a single sampling unit
Continuous sampling	Analysis data that refers to samples collected and stored over a period of time for analysis at a later date. The result obtained is a time-weighted average concentration. There are two forms of continuous sampling - active and passive
Correllation coefficient	A statistical term that gives an indication of the linearity of a set of calibration data. For perfect linearity, the value is $\pm$ 1. As most analyses suffer some degree of random variation, values of close to 1 are acceptable (see regression)
Coulomb	Defined as the quantity of electrical charge (Q) transported by a constant current of 1 amp flowing for 1 sec. [Q = It]
Critical value	An instrument response that triggers an action
Daughter ion	See 'Product ion'
Degenerate modes	The word degenerate refers to physical states having the same energy. In IR spectroscopy the term refers to separate spectral transitions giving rise to spectral bands at the same wavelength.
Degrees of freedom	The number of independent variables used to calculate standard deviation. For every mean calculated, the number is reduced by one
Derivitised	Chemical reaction to create a volatile derivative compound from an involatile analyte, such that the new compound may be separated by gas liquid chromatography. Silicone compounds are frequently used as the derivitising reagent. Alternatively it can refer to the creation of other compounds which have desirable spectroscopic properties such as fluorescence.
Desolvation	The removal of solvent from a sample, prior to it's introduction into a plasma torch

Diode array detector	A spectroscopic detector, consisting of a number of photodiodes, which is capable of recording a complete spectrum of a molecular species, without the need for scanning the wavelength range.
Dipole moment	The measured polarity of a polar covalent bond. It is defined as the product magnitude the charge on the atoms and the distance between the two bonded atoms
Dispersive spectrometer	A spectrometer that separates polychromatic radiation into its component parts before it is incident on the sample. A spectrometer that contains a monochromator as one of its essential components
Distribution coefficient	The quantitative distribution at equilibrium, of a solute (analyte) between two immiscible phases. The higher value of the coefficient, the better the transfer of the solute from the sample (aqueous) to the extracting (organic) phase
Document control system	A system of archiving that ensures that all original material associated with the validation of an analytical method is numbered and stored so as to be available should problems with the method arise in the future
Dynamic range	The range over which the instrument signal varies with respect to analyte concentration.
Electrochemical cell	The combination of a minimum of two electrodes immersed in a solution containing the analyte with an external connection between the electrodes to complete the electrical circuit. There are two types of electrochemical cell - Galvanic (Voltaic) and Electrolytic.
Electrochemical properties	Those electrical properties of a solution that can be used to generate a useful analytical measurement - these are current, voltage, charge and resistance
Electrode	The individual components of an electrochemical cell, through which current passes in the case of electrolytic or galvanic cells, or where potential may be measured when the cells are connected through high impedance voltmeters (eg pH meters)
Electron impact mass spectrometry	The form of mass spectrometry whereby ionisation of analyte molecules occurs resulting from impact with high energy electrons within the mass spectrometer
Electronic transitions	Promotion of electrons from the ground state to another allowable higher energy level, brought about by the absorption of radiation.
Electrophoresis	The transport of electrically charged compounds in solution under the influence of an electric field

Electrothermal vapourisation	Dissociation of inorganic salts and compounds present on the surface of a graphite conductor, to produce neutral atoms, by the rapid electrical heating of the graphite.
Electroyltic cell	A cell where electrical energy is used to force a non-spontaneous chemical reaction to occur - that is, to go in the reverse direction of a 'Galvanic cell'
Elemental fractionation	The variation of measured isotope ratios with time brought about by inappropriate laser ablation
Eluate	An analyte which has eluted from a chromatographic column
Eluent	See 'mobile phase'
Elute	The process whereby substances emerge from a chromatography column following separation
Enriched analyte isotope	see 'Isotope Dilution Mass Spectrometry'
Equivalent weight	An equivalent represents the mass of material containing Avogadro's number of reacting units. Reacting units can be protons or electrons
Evanescent wave	These are formed when sinusoidal waves are internally reflected off an interface at an angle greater than the critical angle so that total internal reflection occurs.
Faraday	The quantity of charge that corresponds to one mole or 6.022 X 1023 electrons. The Faraday constant is 96,485 coulombs/mole of electrons
Fingerprint region of the IR spectrum	The region between approximately 1600 - 625 wavenumbers. This is the part of the spectrum that displays the finest structure, enabling detailed analysis of the spectra to be related to chemical structure.
Fit for purpose	An analytical measurement that satisfies the objective for carrying out the analysis
Fluorescence	A spectroscopic emission process whereby radiation absorbed at one wavelength is emitted at another longer wavelength. Once the source of incident radiation ceases then so also does the flourescent signal
Fortified blanks	A reagent blank solution to which a known quantity of analyte has been added

Fourier Transform (FT)	The conversion of a signal obtained in the frequency domain to one in the time domain
Franck-Condon Principle	This is a rule in spectroscopy and quantum chemistry. The principle states that during an electronic transition, a change from one vbrational energy level to another will be more likely to happen if the two vibrational wave functions overlap more significantly
Frequency	This is defined as the number of cycles of the wave passing a given point in a fixed time (often 1 second, in which case the units would be s^{-1}, also called Hertz, Hz). Frequency is given the Greek symbol v ("nu").
Frits	Small porous discs used to filter out particulate matter or to breakdown a gas stream into small bubbles so as to increase the surface area in contact with a liquid phase.
F-test	A statistical test used to compare two variances
Galvanic (Voltaic) cell	An electrochemical cell which spontaneously produces current when the electrodes are connected
Gas liquid chromatography	A chromatographic separation process, whereby the stationary phase is coated either as a thin layer onto a high surface layer inert substrate or onto the wall of a silica or glass capillary. The mobile phase is a gas which flows over the stationary phase, allowing the vapourised analytes to partition themselves between the two phases
Gas solid chromatography	A chromatographic separation process, whereby the stationary phase is a porous solid packed into a glass or metal column. The mobile phase is a gas which flows over the stationary phase allowing gaseous analytes to spend varying amounts of time within the porous structure, dependent upon the sizes of both the analyte molecules and the pores.
Geiger counter	Geiger-Muller counter - instrument for the detection of ionising radiation (α, β and γ rays) - capable of registering individual particles or photons.
Good laboratory practice	The name given to a set of principles governing the organisation and operation of toxicology studies for food, chemical or pharmaceutical development
Good manufacturing practice	A quality guide relating mainly to the pharmaceutical sector
Grab sampling	Any sampling procedure that collects a single sample at a particular point in time

Gradient elution hplc separation	A predetermined programme that allows two or more solvents to be combined to give a changing mobile phase during the course of an hplc separation
Group frequency region of the IR spectrum	The region of the IR spectrum between approximately 4000 - 1600 wavenumbers. Groups present in the organic molecule exhibit fundamental spectra in this region.
Half-cell	One half of an electrochemical cell - sometimes termed a half-reaction. For example in a Daniell cell, the Cu^{2+}/Cu is one of the half-cells
Horizontal audit	A process carried out by someone from outside the laboratory that examines the elements of the quality system to see if it is working properly. This type of audit is mostly concerned with management and records
Increment	A portion of a material taken from a sampling unit and selected in such a way that it possesses the essential characteristics of the bulk
Inhalable fraction	The particles in the air below 100 µm diameter which can be inhaled into the body through the nose and mouth
Integrity	see 'sample integrity'
Intermediate precision	A measure of precision that incorporates variations in conditions such as different analysts, different equipment and measurements made over a longer timescale. The most appropriate level for the setting of acceptance limits for routine analysis in a quality control laboratory
International conference on harmonisation	This is a project that brings together the regulatory authorities of Europe, Japan and the United States and experts from the pharmaceutical industry in the three regions to discuss scientific and technical aspects of pharmaceutical product registration.
Invasive methods in process analysis	A method that has the potential to modify the sample by the insertion of a probe, side stream etc.
Ion suppression	An effect that can occur when co-eluting compounds, similar to the ion of interest, cause the metabolite to ionise, often in the LC-MS interface, before it gets to the MS detector. This results in a reduced signal, hence the term ion suppression.
Ionic strength	A measure of the total electrolyte concentration in a solution. It is given mathematically by: Ionic strength (μ) = $\frac{1}{2}\sum C_i Z_i^2$ where 'C' represents concentration and 'Z' the charge on the ion
Ionisation potential	The work which must be done, measured in electron-volts, to remove an electron from an atom

ISO 17025	The regulatory standard for chemical testing laboratories, which considers the technical competence of laboratories to carry out specific tests and calibrations
ISO 9001:2000	The international standard covering quality management for companies involved in production or services such as chemical analysis
Isocratic hplc separation	The use of a single chosen mobile phase to perform the separation
Isosbestic point	If both species of a chemical equilibrium absorb and there is some overlap in their absorption spectra, the wavelength where this overlap occurs is termed the isosbestic point
Isothermal gas chromatography	Chromatographic separation carried out at a constant defined temperature
Isotope dilution mass spectrometry	Refers to the use of an enriched isotope of the element of interest as an internal standard.. It involves the addition of a known amount of the enriched isotope to the sample. The addition is made prior to the sample preparation stage such that the enhanced isotope in equilibrated with the sample throughout the whole analysis process. By measuring the isotope ratio of the sample and sample + spike isotope addition and knowing the isotopic ratio of the enhanced addition, the sample concentration can be calculated.
Isotope ratio	The ratio of two isotopes of the same element analysed by ICP-MS
Isotopic fingerprint	The relative abundances of the natural isotopes of an element
IUPAC	International Union of Pure and Applied Chemistry
Jet separator	A component of GC-MS system that allows the separation of heavier analyte molecules from the lighter carrier gas molecules before the molecules enter the mass spectrometer
Labile	Compound that is susceptible to heat - unstable
Laboratory accreditation	Certification by a national body (NAMAS in the UK), that a laboratory is capable of carrying out specific analytical procedures to an acceptable levels of accuracy and precision

Laboratory sample	The portion of the original consignment sent to the laboratory for analysis
Laser ablation	Atomic size fragments emitted from a solid metal surface when a high intensity laser is directed onto that surface.
Lifetime	The time taken for the intensity of the fluorescent emitted light to fall to 1/e of its previous value
Limit of detection	The analyte concentration that gives a signal significantly different to that of the blank/background
Limit of quantitation	The lower limit of analyte concentration for precise quantitative measurement
Linear range	The concentration range over which there is a linear relationship with the instrument signal
Liquid junction potential	The potential created within a salt-bridge which results from the unequal diffusion of the ions on each side of the boundary separating the solutions inside and outside the salt-bridge
Macro levels	Levels between 1 - 100%
Matrix spikes	The addition of a known amount of target analyte to a 'field sample' - a real sample matrix
Mean	The average value from a set of data
Measurement uncertainty	see 'Uncertainty'
Measurement uncertainty budget	An industry term that relates to the components of an analysis that have an effect on the overall estimate of measurement uncertainty and identifies those which are likely to have the greatest impact
Method (analytical)	A combination of techniques used to produce an analytical measurement
Method of least squares	A statistical method used to construct the best straight line fit for a set of calibration data. The method involves minimising the sum of the squares of the residuals. (see residuals)

Method of least squares	A statistical method used to construct the best straight line fit for a set of calibration data. The method involves minimising the sum of the squares of the residuals. (see residuals)
Method validation	The confirmation by examination and provision of objective evidence that the particular requirements for a specific intended use are fulfilled
Michelson interferometer	A device that allows all wavelengths of light to be measured simultaneously, eliminating the need for a wavelength selection device.
Micro levels	Levels between 0.01 - 1%
Mid-IR region	The wavelength region between 2500 - 25000 nm
Millimolar concentrations	A millimolar solution contains a gram molecular mass of solute, divided by 1000, dissolved in water and diluted to 1 dm^3
Miscelles	Molecular aggregates known as surfactants
Mobile phase	A chromatographic term describing the gas or liquid which moves over or through the stationary phase
Molal concentrations	A molal solution contains a gram molecular mass of solute dissolved in 1000 g of solvent
Molar absorptivity	The absorptivity measured when the cell path length is measured in cm and the concentration is molar. The term is given the symbol 'ε' and has units of cm^{-1} $mole^{-1}$ dm^{-1}
Molar concentrations	A molar solution contains a gram molecular mass of solute dissolved in water and diluted to 1 dm^3
Molecular ion	A term in mass spectrometry for the radical ion produced by the collisions inside the mass spectrometer that has the same molecular mass as the original molecule
Molecular ion	The positive ion produced (M+) when an electron collides with a neutral molecule (M) and imparts sufficient energy as to remove an electron from the molecule. It can also be called the 'parent' ion

Molecular vibrations	This occurs when atoms in a molecule are in periodic motion while the molecule as a whole ahs constant translational and rotational motion. A non-linear molecule with 'n' atoms exhibits 3n - 6 normal modes of vibration, whereas a linear molecule exhibits only 3n - 5 normal modes, as rotation about its molecular axis cannot be observed.
Nicolsky equation	A general equation which allows for both the analyte ion and an interfering ion being measured together by an ion selective electrode
Non-invasive methods in process analysis	An analytical measurement obtained by not inserting a measurement device into the process stream
Normal concentrations	A normal solution contains one equivalent per litre of solute
Normal hydrogen electrode	A platinum electrode coated in platinum black, enclosed in a glass tube and over which is passed hydrogen gas at 1 atmosphere pressure. The electrode is immersed in a solution of dilute HCl at unit activity.
Normal phase partition chromatography	The separation that occurs when the stationary phase is polar and the mobile phase is non-polar
Overpotential	The difference between the actual potential where an electrochemical redox reaction occurs and the theoretical potential where it should occur.
Overtones	Extra absorption bands in the IR spectrum at about twice and three times the frequency (or wave number) of the fundamental frequency. These bands are normally found in the near infrared region of the electromagnetic spectrum
Packed gas chromatographic column	A column made from glass or stainless steel tubing (3-8 mm diameter), normally 1-10 m in length. Th column is packed with a suitable packing material
Parent ion	See 'precursor ion'
Partition coefficient	see distribution coefficient
Passive sampling	A form of continuous sampling whereby a sample is collected over a long period of time by the process of natural diffusion of the analyte into a suitable adsorbent. (see continuous sampling)
Performance characteristics	The parameters of an analytical method that define how it will perform. These include sensitivity, precision, accuracy, limit of detection and quantitation, bias, selectivity and dynamic range

Pharmacopoeias	Documented validated methods for use in pharmaceutical analysis
Phosphorescence	A form of luminescence whereby a substance emits radiation at a longer wavelength having absorbed radiation at a shorter wavelength. The wavelength is longer than that expected for fluorescence signal however does continue after the source of incident radiation is removed (see fluorescence)
Photo diode array detector	See 'diode array detector'
Photon	The energy of a unit of radiation, it is related to both frequency and radiation
Plackett-Burman	An experimental design technique used to test the impact that a change in a variable will have on the results of an experiment
Pocess analytical chemistry	The tailoring of laboratory-based analytical techniques to allow their direct use in the manufacturing environment
Polarography	A form of voltammetry using mercury, mainly in the form of reproducible drops, as the working electrode. (see Voltammetry)
Population standard deviation	The measurement of the standard deviation of the noise from a signal output, can be estimated as the polulation SD, when more than 30 measurements of peak to peak noise are recorded.
Potentiostatic circuit	An electronic circuit for electrolytic measurements involving 3 electrodes - reference, working and auxiliary. The potential at the working electrode is held at a constant value with respect to the reference electrode. The current generated flows between the working and the auxiliary electrodes. A plot of current flow is recorded versus the potential at the working electrode, without any disturbance caused by appreciable solution resistance creating an iR drop.
Precision	The scatter of the measured values
Precursor ion	The molecular ion produced following initial ionisation in a tandem MS-MS system.
Principal component analysis	A mathematical and statistical technique to identify patterns of data in a complex high dimension data set
Probability	The extent to which something is probable

Procedure (analytical)	The set of detailed instructions to carry out an analysis
Product ion	Ions produced by the dissociation of molecular, precursor or parent ions in a tandem MS-MS system. Also known as 'daughter ions'.
Proficiency testing	A scheme aiming to test the competence of the analysts working within an analytical laboratory
Propogation of error	The sources of error associated with an analysis (see measurement uncertainty)
Protocol	The agreed set of tests to be carried out to validate an analytical method
Qualitative analysis	Identifies what chemicals, substances, ions, atoms or molecular functional groups are present in the sample to be analysed
Quality	The totality of features and characteristics of a product or service that bear on its ability to satisfy stated or implied needs
Quality assurance	The planned system of activities whose purpose is to provide assurance that the quality control system is actually effective
Quality control	Planned activities designed to provide a quality product
Quality management	The system set up to manage the quality policy, identify quality objectives and plan the processes and procedures required to achieve the standards of quality expected by the customer or the regulator
Quality manual	The combination of documentation stored in a single folder which expresses the quality management policy of an analytical laboratory
Quantitative analysis	Measures the quantity of a substance, compound, ion, atom or molecular grouping which is present in the sample presented for analysis
Quantum yield	The fraction of excited molecules that lose their energy by the emission of fluorescent radiation. It is usually expressed as a number between 0 - 1
Random error	Errors that arise from uncertainties in a measurement that are unknown and cannot be controlled. The result is a scatter of replicate measurements that can only be assessed by statistical tests
Rayleigh scattering	Scattering mechanism, in which the photon–molecule collisions are elastic ie. do not involve any exchange of energy. Scattered photons have the same wavelength as the incident photons.

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Real-time sampling and analysis	Refers to any sampling system where the sample is taken and passed directly to an analyser to provide immediate analytical results.
Recovery studies	The addition of a known quantity of an analyte to a sample and the measurement of the analyte both before and after the addition
Reference electrode	Reference electrodes are half cells whose potential is independent of the measurement conditions and which are inert to changes in those conditions during the course of a measurement
Reference materials	A homogeneous material or substance, one or more properties of which are sufficiently well documented so that it may be used to calibrate an apparatus, assess an analytical method or assign values to materials
Regression (line of)	A statistical term that relates to a line showing how 'y' varies with 'x' for a set of chosen values. For a perfect correlation between 'y' and 'x' the value of regression (r) will be 1. (see correlation coefficient)
Relative retention ratio	The ratio of the adjusted retention of the analyte to that of a standard or reference substance
Relative standard deviation	Standard deviation expressed as a % of the mean value for that set of data
Repeatability	Defines precision data obtained over a short time interval using the same operating procedure. The level of precision expected from a set of replicate determinations
Representative sample	A portion of a material taken from a consignment and selected in such a way that it possesses the essential characteristics of the bulk
Reproducibility	Defines precision data obtained from collaborative studies within different laboratories and over a much longer timescale. It will reflect variation from a wider range of sources
Residuals	The positive and negative differences in 'y' values resulting from the production of a 'best fit' calibration graph
Resonance wavelength	The energy corresponding to the most probable electronic transition which is normally from the ground state to the lowest excited state and *vice versa*
Respirable fraction	The mass fraction of inhaled particles that penetrates the uncillated airways of the lung

Reversed phase partition chromatography	The separation that occurs when the stationary phase is comparatively non-polar and the mobile phase is polar
Rhoracic fraction	The mass fraction of inhaled particles penetrating the respiratory system beyond the larynx
Robustness	The measure of the capacity of a method to remain unaffected by small but deliberate variations in method parameters. It provides an indication of the reliability of a method during normal usage
Ruggedness	see Robustness
Sample integrity	Integrity in this context, refers to the structure and composition of the sample being the same when analysed as when it was taken
Samples for analysis	Replicate portions of the 'test sample' (see Test sample)
Sampling plan	A predetermined procedure for the selection, withdrawal, preservation, transportation and preparation of samples taken for analysis
Sampling procedure	The succession of steps set out in a specification, which ensures that the sample eventually taken for analysis shall possess the essential characteristics of the bulk
Sampling unit	A physically separate part of a batch or consignment from which one of more samples or sample increments will be taken
Scattered light	Scattered light refers to the phenomenon whereby the photon of incident light collides with a molecule in the sample cuvette and as a result emerges in a new direction, such that it does not reach the detector
Scintillation counter	A device in which light flashes are produced by a scintillator when exposed to ionising radiation. The emitted radiation is collected and measured by a photomultiplier
Selective ion monitoring	A mass spectrometry detection system used with gas and liquid chromatography, whereby only ions of selected mass/charge ratios are detected to produce a chromatogram.
Selectivity	The ability to measure the analyte in the presence of other potentially interfering substances that may be present in the matrix. It is sometime combined with another term such as index or coefficient
Sensitivity	The change in measured signal for unit change in concentration. Usually measured as the slope of the calibration graph

Shewart charts	A simple type of quality control chart. The measured value is plotted on the 'y' axis against time of successive measurements on the 'x' axis
Single ion monitoring	see 'Selective ion monitoring'
Soft ionisation techniques	Low energy ionisation techniques used in some aspects of mass spectroscopy.
Solid phase extraction	Solid-phase extraction (SPE) is a powerful sample pre-treatment procedure, particularly prior to analysis by high performance or gas-liquid chromatography. It involves the exhaustive removal of chemical substances from flowing samples (often aqueous), via retention onto a solid sorbent contained in a preformed cartridge.
Specific analytical technique	An analytical technique which only measures or detects a given analyte
Specificity	The ability to assess unequivocally the analyte in the presence of compounds that maybe expected to be present. Defined by IUPAC as the ultimate in selectivity (see selectivity)
Spiked samples	The quantity of analyte added to a sample matrix as part of a recovery study (see recovery study)
Splitter	The device used in capillary chromatography, that allows only a small proportion of the vapourised sample to pass onto the separating column
Stable isotope dilution	See 'Isotope Dilution Mass Spectrometry' but with the use of stable isotopes
Standard deviation	A statistical measure based upon the spread of a set of replicate data - it is an estimate of precision
Standard deviation of the mean	Sometimes referred to as the standard error of the mean. A statistical value obtained by dividing the standard deviation by the square root of the number of pieces of data used to calculate the standard deviation. It provides a measure of the uncertainty involved in estimating the true value(μ) from the calculate mean value
Standard operating procedure	Unambiguous instructions on how to carry out a wide range of operations. In the context of analytical science it would define the setting up and operation of specific instrumentation together with the carrying out of the full analytical method
Stationary phase	The phase in a chromatographic separation that remains stationary

Stokes lines	Scattered photons that have a higher wavelength (lower energy) than the incident light
Stray light	Any radiation reaching the detector which did not form part of the incident beam
Sub-sampling	Reduction in the size of samples or composite samples whilst retaining sample representation
Systematic error	These are measurable errors which in theory have a definite value and thus can be allowed for during an analysis
Technique (analytical)	A chemical or physical process by which a separation or a measurement is carried out.
Temperature programming	Gas chromatographic analysis carried out at a pre-programmed set of temperatures, from low at the start to high at the end
Test sample	A sample produced by sub-division representatively, the 'laboratory sample'. This will subsequently be used to provide replicate samples for analysis. (see Laboratory sample, and Sample for analysis)
Thermal desorption	The use of heat and a flow of gas, to drive adsorbed volatile organic compounds from the adsorbent, directly onto a gas chromatography column
Thin-layer chromatography	A form of liquid chromatogaphy whereby the stationary phase is coated onto a flat sheet of glass or plastic. Samples to be separated are spotted near the base of the plate and separation occurs by the mobile phase moving up or along the plate by capillary action.
Thoracic fraction	The mass fraction of inhaled particles penetrating the respiratory system beyond the larynx
Time mass pair	Data from an LC-MS profile saved and displayed as a peak value, associated with a retention time and mass.
Time-weighted average	An analytical result where the total concentration of the analyte as measured is divided by the time over which the sample was collected.
Total internal reflectance	An optical phenomenon that occurs when a ray of light strikes a medium boundary at an angle larger than the critical angle with respect to the normal to the surface. If the refractive index is lower on the other side of the boundary no light can pass through, so effectively all of the light is reflected. The critical angle is the angle of incidence above which the total internal reflection occurs.

Total ion monitoring	A mass spectrometry detection system used with gas and liquid chromatography, whereby all of the ions produced in the mass spectrometer are detected and used to produce the chromatogram
Total ionic stength adjustment buffers	A complex buffer which allows the ionic strength to be maintained at a constant value through a range of measurements. These buffers often contain complexing agents to prevent losses of analyte ion due to speciation effects.
Trace levels	Levels between 0.00001 - 0.01% (0.1 - 100 ppm)
Traceability	The property or result of a measurement whereby it can be related to appropriate national or international standards through an unbroken chain of comparisons
Transducer	A type of detector that converts various types of chemical and physical quantities into electrical signals such as current and voltage.
Transmittance	The ratio of transmitted radiation passing through a sample to that incident on the sample
True value	The true value of an analyte concentration is only known for a standard solution prepared from pure materials
Trueness	The closeness of agreement between the average value obtained from a large set of test results and an accepted reference value
t-test	A statistical test used to compare two mean values
Turbimetry	A technique, whereby a solution contains suspended particles and scatters, rather than absorbing, the incident radiation
Ultrasonic nebulisation	The process whereby the nebuliser uses an ultrasonic generator to disrupt the liquid/air interface such that the resulting aerosol is swept into the ICP torch by a stream of inert gas, where it is ionised and subsequently analysed by MS.
Ultra-trace levels	Levels below 0.00001% (less than 0.1 ppm)
Uncertainty (measurement)	A parameter associated with the results of a measurement that characterises the dispersion of the values that could reasonably be attributed to the measurement
Uncertainty principle	It is impossible to determine with accuracy both the position and the momentum of a particle simultaneously. The more accurately the position is known, the less accurately can the momentum be determined. The principle arises due to the dual particle/wave nature of matter

Unit activity	See activity. The concentration of the solution in mol/dm^3 to give a solution having an activity = 1
Variance	The square of the standard deviation
Venturi effect	The escape of gas through a narrow constriction in the nebulizer, causes a pressure reduction at that point. This reduced pressure, at the tip of the nebulizer, in turn draws liquid up the capillary tube without the constriction in the nebulizer, causes need for a peristaltic pump.
Verification checks	S+B119imple performance checks to ensure a specified requirement has been fulfilled
Vertical audit	A process carried out by someone from outside the laboratory that examines individual pieces of work, selected at random
Voltaic cell	See 'Galvanic cell'
Voltammetry	An electrolytic analytical technique where the potential (energy source) is scanned between two set values at a micro electrode. At a specific potential, a portion of the analyte will be reduced or oxidised with the consequential flow of current. The current increases linearly with increase in potential in accordance with Ohm's Law. The total current flow is dependent upon diffusion of the analyte to the working electrode and at low concentrations is proportional to the analyte concentration.
Wavelength	This is defined as the distance from one maximum of the vibrational amplitude to the next: it is always given the Greek letter λ (“lamda”).
Wavenumber	This is defined as the reciprocal of the wavelength, i.e. the number of vibrations in a given distance (usually 1 cm), in which case the units are cm^{-1}. These units are mostly used in infra-red spectroscopy. Its symbol is (confusingly, perhaps nu-bar)
Working range	See dynamic range
Xenobiotic metabolism	The metabolism of foreign compounds, from drugs, pollutants to pesticides,
X-ray diffraction	Pattern obtained by the scattering of X-rays by crystals. Can be used to identify crystal structures
X-ray fluorescence	X-rays emitted by a sample following irradiation by a beam of X-rays, that are characteristic of the atoms involved. These fluorescent X-rays are at a longer wavelength than those of the initial irradiating beam