

Forensic Toxicology: Terms and Definitions

DRAFT



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Forensic Toxicology: Terms and Definitions

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Foreword

This document contains a list of terms and definitions to be used by the Toxicology Consensus Body of the American Academy of Forensic Sciences (AAFS) Academy Standards Board (ASB) and the Forensic Toxicology Subcommittee of the Organization of Scientific Area Committees (OSAC) for Forensic Science ~~and the Toxicology Consensus Body of the American Academy of Forensic Sciences (AAFS) Academy Standards Board (ASB)~~ for documents developed for forensic toxicology. Some terms may be used differently in other disciplines. Using this technical report as a normative reference in forensic toxicology standards, guidelines, and best practice recommendations drafted by the OSAC and developed by the ASB will negate the need to relist and define terms that are already contained within this report.

The overall intent of this technical report is to include terms used in various standards, guidelines, and best practice recommendations for consistency and consolidation. Terms and definitions needed at a detailed level for a specific standard, guideline, or best practice recommendation are defined within that document. As these documents go through the revision process, terms and definitions that apply at the higher level will be migrated from individual documents to this technical report. If a conflict exists between a definition in this report and a published ASB document, the definition in this document prevails.

The AAFS established the ASB in 2015 with a vision of safeguarding Justice, Integrity, and Fairness through consensus-based American National Standards. To that end, the ASB develops consensus-based forensic standards within a framework accredited by the American National Standards Institute (ANSI) and provides training to support those standards. ASB values integrity, scientific rigor, openness, due process, collaboration, excellence, diversity, and inclusion. ASB is dedicated to developing and making freely accessible the highest quality documentary forensic science consensus Standards, Guidelines, Best Practice Recommendations, and Technical Reports in a wide range of forensic science disciplines as a service to forensic practitioners and the legal system.

ASB is accredited by the American National Standards Institute (ANSI) according to ANSI's "Essential Requirements: Due Process Requirements for American National Standards."¹ ASB documents are developed by volunteers working in Consensus Bodies (CBs) and Working Groups (WGs) that conform to ANSI requirements of openness, transparency, due process, and consensus.

This document was prepared, revised, and finalized as a technical report by the Toxicology Consensus Body of the AAFS Standards Board.

Questions, comments, and suggestions for the improvement of this document can be sent to ASB Secretariat, asb@aafs.org or 410 N 21st Street, Colorado Springs, CO 80904.

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Forensic Toxicology: Terms and Definitions

1 Scope

This document provides terms and definitions for use in standards, guidelines, and best practice recommendations developed for forensic toxicology. The terms in this technical report apply to documents published by the ASB Toxicology Consensus Body.

2 Normative References

There are no normative references for this document.

3 Terms and Definitions

The following terms and definitions apply to standards, guidelines, and best practice recommendations developed for forensic toxicology and published by the ASB Toxicology Consensus Body.

3.1

accuracy ^[4]

closeness of agreement between a measured quantity value and a true quantity value of a measurement

3.2

administrative review ^[3]

evaluation of records to verify consistency with administrative policies and editorial correctness

3.3

analyte

chemical substance to be identified and/or measured

3.4

analytes of interest

drugs, drug metabolites, and other chemicals included within the ~~test method's~~analytical scope of a test method

3.5

analytical run

“batch”

set of ~~standards~~case samples, controls, and/or case samples~~calibrators~~ that are contemporaneously prepared and/or analyzed in a particular sequence

3.6

analytical scope

selection of drugs, drug metabolites, and other chemicals covered in an analytical ~~testing~~scheme~~strategy~~

3.7**analytical sensitivity**

lowest amount of an analyte that can be reliably measured in a specimen by a laboratory test; may be a decision point, a limit of detection, or a lower limit of quantitation

3.8**analytical strategy** ^[3]

choice of methods and the sequence of analysis

3.9**bias (cognitive)** ^[6]

set of influences that may affect the reliability and validity of one's observations and conclusions

3.10**bias (measurement)**

estimate of systematic measurement error, calculated as the difference between the mean of several measurements under identical conditions, to a known "true" value

3.11**bias (statistical)** ^[6]

systematic tendency for estimates or measurements to be above or below their true values

NOTE 1: Statistical bias arises from systematic as opposed to random error.

NOTE 2: Statistical biases can occur in the absence of prejudice, partiality, or discriminatory intent.

3.12**blank matrix sample**

biological fluid (e.g., blood, urine, bile, serum, vitreous humor, oral fluid), tissue, or synthetic substitute without target analyte or internal standard

3.13**breath alcohol program**

organizational structure including policies, procedures, responsibilities, and resources necessary for implementing core breath alcohol activities

NOTE: The Breath Alcohol Program includes, but may not be limited to, requirements or specifications for reference materials, training of operators, maintenance and calibration of instrumentation, the evidential breath alcohol test sequence, and record retention.

3.14**calibration** ^[4 (modified)]

operation that, under specified conditions, establishes a relationship between the **quantity value** concentration of analyte and the corresponding instrument response

3.15**calibration model**

mathematical model that represents the relationship between the known concentration of analyte and the corresponding instrument response

3.16**calibrator** ^[1]

measurement standard used in calibration

3.17**carryover**

detection of unintended analyte signal in a sample after the analysis of a positive sample containing that analyte

3.18**case file** ^[3]

forensic service provider's collection of all records detailing the forensic process including reports related to a case

3.19**certified reference material** ^[1]**CRM**

reference material characterized by a metrologically valid procedure for one or more specified properties, accompanied by a certificate that provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability

3.20**chain of custody** ^[3]

chronological record of the transfer, handling, and storage of an item from its point of collection to its final return or disposal

3.21**chromatography** ^[5]

physical method of separation in which the components to be separated are distributed between two phases, one of which is stationary (stationary phase) while the other (the mobile phase) moves in a definite direction

3.22**concurrently analyzed**

analyzed at or close to the same time under the same analytical conditions (i.e., same instrument and instrumental parameters)

3.23**consensus result**

value that serves as an agreed-upon reference for comparison that is based on the results of laboratories participating in the proficiency test

3.24**control**

material of known composition that is analyzed along with unknown sample(s) in order to evaluate the performance of an analytical procedure

3.25**court-ordered toxicological testing**

analysis of specimens from subjects involved in probation and parole, drug courts, or child protective services to determine the presence (or absence) of chemical substances and their effects on the average individual

3.26**customer** ^[3 (modified)]

authority, organization, [and](#)/or person(s) requesting forensic toxicology services

3.27**data**

see *observation*

3.28**decision point**

administratively defined cutoff concentration that is at or above the method's analytical detection [limit](#)

3.29**diagnostic ion**

MS or MS/MS molecular ion or fragment ion whose presence and relative abundance are characteristic of the targeted analyte

3.30**drug-facilitated crime****DFC**

when an individual is victimized while mentally or physically incapacitated due to the effects of ethanol and/or other drugs

3.31**examination** ^[3 (modified)]

part of the forensic toxicology process consisting of the analysis of specimen(s) and the interpretation of observations from the analysis

3.32**high-resolution mass spectrometry****HRMS**

[acquisition of data using a](#) mass spectrometer ~~instrument~~ that can give at least 10,000 nominal mass resolving power at the full width of the peak at half its maximum height (FWHM) for the compound of interest

3.33**human performance toxicology**

analysis of specimens for driving while impaired cases, drug-facilitated crimes, and other impairment cases to determine the presence (or absence) of chemical substances and their effects on the average individual

**3.34
identification** ^[3]

Assignment to the most specific class attainable

NOTE: In forensic toxicology, identification refers to determining the presence of drugs, chemicals, or toxins within a biological sample.

**3.35
immunoassay**

analytical ~~test~~ that ~~rely~~ relies upon the interaction between antibodies and antigens (e.g., drugs or drug metabolites)

**3.36
interferences**

~~non-targeted~~ compounds (e.g., matrix components, other drugs, metabolites, internal standard, and impurities), which may impact the ability to detect, identify, or quantitate a targeted analyte

**3.37
interpretation**

explanations for the observations and calculations

NOTE: In forensic toxicology, interpretations are ~~the~~ considered reported findings.

**3.38
ion ratio**

in mass spectrometry, the ratio of the instrument responses between two previously identified diagnostic ions

**3.39
ionization**

physicochemical process of producing a gas-phase ion

NOTE: This typically occurs within the ion source in the mass spectrometer. Several mechanisms of ionization exist, such as chemical and electron ionization.

**3.40
isomers** ^[5]

compounds that have the same elemental formula but have different structural configurations and ~~hence~~ thus different physical and/or chemical properties

**3.41
laboratory-developed test method**

~~Type~~ type of non-standard test method designed and used within a single laboratory or laboratory system

**3.42
limit of detection****LOD**

estimate of the lowest concentration of an analyte in a sample that can be reliably differentiated from blank matrix and meets identification criteria for the analytical method

3.43**low-resolution mass spectrometry****LRMS**

[acquisition of data using a mass spectrometer instrument](#) limited to nominal mass resolution measurements

3.44**lower limit of quantitation****[LLOQ](#)**

estimate of the lowest concentration of an analyte in a sample that can be reliably measured with acceptable bias and precision

3.45**mass spectrometry ^[5]****MS**

study of matter through the formation of gas-phase ions that are characterized using mass spectrometers by their mass, charge, structure, and/or physicochemical properties

3.46**matrix**

specific biological fluid ~~or tissue~~ (e.g., blood, plasma, serum, urine, oral fluid, vitreous fluid~~), hair, and tissue~~), ~~or non-human/animal substitute~~

[3.47](#)**[measurement uncertainty](#)****[\(uncertainty of measurement\)](#)**

[estimate of the potential variability of a quantitative measurement based on the information known about the measurand and the measurement method](#)

[3.473.48](#)**method development**

process by which analytical parameters are established for a non-standard test method, laboratory-developed test method, or standard test method used outside its intended scope (or otherwise modified) that considers sample preparation, instrumental conditions, interpretation of observations, data, or calculations, and metrological traceability

[3.483.49](#)**method of standard addition****MSA**

quantitative procedure by which known concentrations of target analyte are added to multiple aliquots of the case sample(s)

[3.493.50](#)**~~3.50~~****method validation**

process of performing a set of experiments to establish objective evidence that a non-standard test method, laboratory-developed test method, or standard test method used outside its intended scope (or otherwise modified) is fit for purpose and to identify limitations under normal operating conditions

~~3.51~~[3.523.51](#)**method verification**

process by which a laboratory establishes objective evidence of its ability to use [a non-standard test method, laboratory-developed test method, or](#) standard test method within its intended scope to achieve the method's defined performance specifications

~~3.533.52~~**metrological traceability** ^[1]
(measurement traceability)

property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty

~~3.543.53~~**molecular ion** ^[5]

ion formed by the removal of one or more electrons from a molecule to form a positive ion or the addition of one or more electrons to a molecule to form a negative ion

~~3.553.54~~**MSⁿ** ^[5]

multiple-stage mass spectrometry experiments designed to record product ion spectra where n is the number of product ion stages (nth-generation product ions)

~~3.563.55~~**multiple reaction monitoring** ^[5]
MRM

application of selected reaction monitoring to multiple product ions from one or more precursor ions

~~3.573.56~~**nominal mass** ^[5]

mass of a molecular ion or molecule calculated using the isotope mass of the most abundant constituent element isotope of each element rounded to the nearest integer value and multiplied by the number of atoms of each element

~~3.583.57~~**nominal quantity value** ^[4]

rounded or approximate value of a characterizing quantity of a measuring instrument or measuring system that provides guidance for its appropriate use

~~3.593.58~~**non-regulated workplace drug testing**

non-federally mandated analysis of specimens from employees to determine the presence (or absence) of specific chemical substances and their effects on the average individual

~~3.603.59~~**non-standard test method**

defined test procedure that is used to generate test results and published by an entity other than a national or international standards development organization

NOTE: Non-standard test methods include those from vendors, scientific journals, standard practices or guides, and laboratory-developed methods.

3.613.60

observation (data) [3 (modified)]
results of analysis of items

NOTE: An observation can result from human-perception-based analysis, instrumental analysis, or a combination of the two.

3.623.61

opinion [6]
view, judgment, or belief that considers other information in addition to observations, data, calculations, and interpretations

3.633.62

postmortem toxicology
analysis of specimens from decedents in medicolegal death investigations to determine the presence (or absence) of chemical substances and their effects on the average individual

3.643.63

precision
measure of the closeness of agreement between a series of measurements obtained from multiple samplings of the same or similar homogenous samples

3.653.64

precursor ion [5 (modified)]
ion that reacts to form particular product ions or undergoes specified neutral losses

3.65

presumptive positive
analytical result that, on its own, does not achieve the minimum points for the identification of a substance

NOTE See ANSI/ASB Standard 113: Standard for Identification Criteria in Forensic Toxicology for a complete discussion of identification points.

3.66

product ion [5 (modified)]
ion formed as the product of a reaction involving a precursor ion

3.67

proficiency testing [2 (modified)]
evaluation of participant performance against pre-established criteria by means of interlaboratory comparison

3.68

qualitative method
assay designed to determine the presence (or absence) of an analyte within a sample relative to an established threshold

3.69**quantitative method**

assay designed to measure the concentration of an analyte within a sample

3.70**reference material** ^[4]

material, sufficiently homogenous and stable with reference to specified properties, which ~~have~~[has](#) been established to be fit for its intended use in a measurement or in examination of nominal properties

3.71**regression**

set of statistical processes for estimating the relationships between a dependent variable and one or more independent variables (e.g., linear, quadratic, simple, etc.)

3.72**repeatability** ^[4, (modified)]

measurement precision under a set of conditions that includes the same measurement procedure, same operators, same measuring system, same operating conditions, ~~same conditions~~, and same location, and replicate measurements on the same or similar objects over a short period of time

3.73**reporting range**

concentrations that can be reliably measured by an analytical procedure that will be reported per the ~~Program's~~ specifications [of the laboratory, breath alcohol program, or its customers.](#)

3.74**reproducibility**

measurement precision under a set of conditions that includes different locations, operators, measuring systems, and replicate measurements on the same or similar objects

~~**3.75**~~**results**~~[3.76](#)~~[3.75](#)

the product of the forensic service provider

NOTE 1: The term is broad and includes observations, calculations, interpretations, and opinions.

NOTE 2: In forensic toxicology, test/calibration results (observations, calculations, and interpretations) are often separated from opinion results.

~~**3.77**~~~~**screening method**~~

~~assay designed to rule out the presence of analytes or to suggest their presence, thereby indicating further testing may be warranted~~

~~[3.78](#)~~[3.76](#)

selected ion monitoring ^[5]**SIM**

operation of a mass spectrometer in which the abundances of ions of one or more specific m/z values are recorded rather than the entire mass spectrum

[3.793.77](#)**selected reaction monitoring** ^[5]**SRM**

data acquired from one or more specific product ions corresponding to m/z selected precursor ions recorded via two or more stages of mass spectrometry

[3.803.78](#)**specificity**

ability of a method to distinguish between the targeted analyte and other non-targeted substances

[3.813.79](#)**specimen**

matrix sample collected from a specific origin for toxicological analysis (e.g., femoral or cardiac blood, left versus right eye vitreous fluid, and liver, brain, or kidney)

[3.823.80](#)**stability**

analyte's resistance to chemical change in a matrix under specific conditions for given time intervals

[3.833.81](#)**standard test method**

defined test procedure published by national or international standards development organizations that is used unmodified to generate test results

NOTE: Examples of standard test methods include, but are not limited to, identification, measurement, and evaluation of one or more qualities, characteristics, or properties. Standard test methods include precision and bias statements.

[3.843.82](#)**tandem mass spectrometry** ^[5]**MS/MS**

acquisition and study of the spectra of the product ions or precursor ions of m/z selected ions, or of precursor ions of a selected neutral mass loss

[3.853.83](#)**technical review** ^[3]

evaluation of all supporting records from the examination and the report, if prepared, to evaluate observations and assess whether there is an appropriate and sufficient basis for any opinions

[3.863.84](#)**upper limit of quantitation****ULOQ**

highest concentration of an analyte in a sample that can be reliably measured with acceptable bias and precision

Annex A (informative)

Bibliography

The following bibliography is not intended to be an all-inclusive list, review, or endorsement of literature on this topic. The goal of the bibliography is to provide examples of publications addressed.

- 1] International Organization for Standardization (ISO). "ISO/IEC 30:2015, Reference Materials – Selected Terms and Definitions". (Geneva, Switzerland: ISO).²
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- 5] Murray, K.K., R.K. Boyd, M.N. Eberlin, G.J. Langley, L. Li, Y. Naito. "Definitions of terms relating to mass spectrometry (IUPAC Recommendations 2013)." Pure and Applied Chemistry 2013, 85 (7), 1515-1609.⁶

[6\] OSAC Lexicon Preferred Terms.](#)⁷

² <https://www.iso.org/standard/46209.html>

³ <https://www.iso.org/standard/80864.html>

⁴ <https://www.iso.org/standard/69732.html>

⁵ [cb0ef43f-baa5-11cf-3f85-4dcd86f77bd6 \(bipm.org\)](https://www.bipm.org/pubs/2010/guides/gum/gum100-2008-gum1995-with-minor-corrections/)

⁶ <https://publications.iupac.org/pac/pdf/2013/pdf/8507x1515.pdf>

⁷ <https://www.nist.gov/glossary/osac-lexicon#top>

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