Data Glossary

The purpose of this data glossary is to provide a reference for terms used in the analytical analysis of polychlorinated biphenyl (PCB) congeners, utilizing high resolution gas chromatography/high resolution mass spectrometry/ (HRGC/HRMS) methods. The definitions and equations provided are specific to HRGC/HRMS methods used in the analysis of chlorinated biphenyl congeners.

Acceptance criteria - specific limits placed on characteristics of an item, process, or service defined in requirements documents.

Analyte - Any of 209 chlorinated biphenyl (CB) congeners.

Bias - the systematic or persistent distortion of a measurement process that causes errors in one direction (i.e., the expected sample measurement is different from the sample's true value).

Calibration standard (CAL) - A solution prepared from a secondary standard and/or stock solutions and used to calibrate the response of the HRGC/HRMS instrument.

Calibration verification standard (VER) - The mid-point calibration standard (CS-3) that is used to verify calibration.

CB—chlorinated biphenyl congener. One of the 209 individual chlorinated biphenyl congeners determined using Method 1668A.

CAS # (CASRN)---- Chemical Abstracts Service Registry Number. CAS Registry Numbers are unique identifiers for chemical compounds.

Congener Number---A numbering system from 1-209, which uniquely identifies each of the 209 chlorinated biphenyl congeners. This numbering system was formerly referred to as the BZ and IUPAC number and remains identical to the numbering system published by Ballschmiter et al., 1992 (BZ #'s).

Data quality assessment (DQA) - a statistical and scientific evaluation of the data set to determine the validity and performance of the data collection design and statistical test, and to determine the adequacy of the data set for its intended use.

Data quality objectives (DQOs) - qualitative and quantitative statements that clarify study objectives, define the appropriate type of data, and specify tolerable levels of potential decision errors that will be used as the basis for establishing the quality and quantity of data needed to support decisions.

Data usability - the process of ensuring or determining whether the quality of the data produced meets the intended use of the data.

Data validation – an analyte- and sample-specific process that extends the evaluation of data beyond method, procedural, or contractual compliance (i.e., data verification) to determine the analytical quality of a specific data set.

Data validation qualifier – code applied to the data by a data validator to indicate a verifiable or potential data deficiency or bias.

Data verification – the process of evaluating the completeness, correctness, and conformance/compliance of a specific data set against the method, procedural, or contractual requirements.

Equipment Blank or Rinsate Blank - A blank consisting of analyte-free media which has been used to rinse the sampling equipment. It is collected after completion of equipment decontamination and prior to sampling. This blank is useful in documenting adequate decontamination of sampling equipment and determining the impact of any contamination that may be present on the associated investigation samples.

Estimated detection limit (EDL) — The sample specific estimated detection limit (EDL) is the concentration of a given analyte required to produce a signal with a peak height of at least 2.5 times the background signal level. This concentration is determined by measuring the noise height of the two quantitation ions for a given congener at the region of the SICP where the congener is expected to elute, converting this height into area based on the associated internal standard area, and taking the internal standard concentration, internal standard area, initial calibration average RRF, minimum signal-to-noise factor, and sample weight/volume into account.

Estimated minimum level (EML)—The lowest concentration at which a CB can be measured reliably with common laboratory interferences present. EMLs for Method 1668A are provided in Table 2 of the Method. EMLs should be routinely achievable by laboratories running the method.

False negative or false acceptance decision error - the error that occurs when a decision maker accepts a result as true when it is actually false. Also referred to as a Type II error.

False positive or false rejection decision error - the error that occurs when a decision maker rejects a result when it actually is true. Also referred to as a Type I error.

Field blank—An aliquot of reagent water or other reference matrix that is placed in a sample container in the laboratory or the field, and treated as a sample in the following respects, including exposure to sampling site conditions, storage, preservation, and all analytical procedures. However, a field blank is not used to rinse the sampling equipment. The purpose of the field blank is to determine if the field or sample transporting procedures and environments have potentially contaminated the associated investigation samples.

Field Replicates - Independent samples that are collected as close as possible to the same point in space and time. They are two separate samples taken from the same source, stored in separate containers, and analyzed independently. These replicates are useful in documenting the overall precision of the sampling and analytical process. This definition is presented to distinguish a field replicate from a field duplicate. A field duplicate is a split of a well mixed homogenized sample.

High Resolution Gas Chromatography (HRGC) - A gas chromatograph is an instrument which is used to separate the components of a mixture. A high resolution GC provides the capability of separating similar substances in complex mixtures.

High Resolution Mass Spectrometry (HRMS) - A mass spectrometer is an instrument that measures the masses of individual molecules or molecular fragments that have been converted into ions, i.e., molecules or fragments that have been electrically charged. Mass spectrometers use the difference in mass-to-charge ratio (m/z) of ionized molecules or fragments to separate them from each other.

Internal standard—a labeled compound used as a reference for quantitation of other labeled compounds and for quantitation of native CB congeners other than the congener of which it is a labeled analog. See Internal standard quantitation.

Internal standard quantitation—A means of determining the concentration of (1) a naturally occurring (native) compound by reference to a compound other than its labeled analog and (2) a labeled compound by reference to another labeled compound.

IPR—Initial precision and recovery; four aliquots of a reference matrix spiked with the analytes of interest and labeled compounds and analyzed to establish the ability of the laboratory to generate acceptable precision and recovery. An IPR is performed prior to the first time this Method is used and any time the Method or instrumentation is modified.

Isotope Dilution - An analytical technique where a compound is determined in reference to the same compound in which one or more atoms has been isotopically enriched. This technique results in extremely accurate identification and quantitation. It also allows for determination of matrix effects on a sample specific basis.

Isotope dilution quantitation—A means of determining a naturally occurring (native) compound by reference to the same compound in which one or more atoms has been isotopically enriched. In Method 1668A, all 12 carbon atoms in the biphenyl molecule are enriched with carbon-13 to produce 13C12-labeled analogs of the chlorinated biphenyls. The 13C12-labeled CBs are spiked into each sample and allow identification and correction of the concentration of the native compounds in the analytical process.

Laboratory control sample (LCS)—See Ongoing precision and recovery standard (OPR) **-** A known matrix spiked with compound(s) representative of the target analytes. This is used to document laboratory performance

Laboratory blank—See Method blank

Laboratory reagent blank—See Method blank

Matrix Duplicate - An intralaboratory split sample that is used to document the precision of a method in a given sample matrix.

Matrix Spike - An aliquot of sample spiked with a known concentration of target analyte(s). The spiking occurs prior to sample preparation and analysis. A matrix spike is used to document the bias of a method in a given sample matrix.

Matrix Spike Duplicate - Intralaboratory split samples spiked with identical concentrations of target analyte(s). The spiking occurs prior to sample preparation and analysis. They are used to document the precision and bias of a method in a given sample matrix.
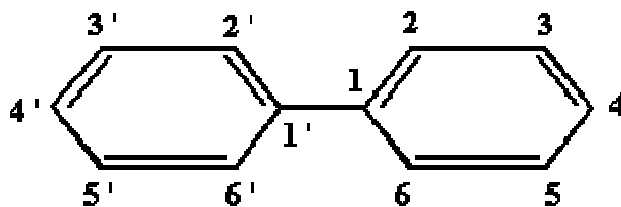
Method blank—an aliquot of reagent water that is treated exactly as a sample including exposure to all glassware, equipment, solvents, reagents, internal standards, and surrogates that are used with samples. The Method blank is used to determine if analytes or interferences are present in the laboratory environment, the reagents, or the apparatus.

Minimum level of quantitation (ML)—The level at which the entire analytical system must give a recognizable signal and acceptable calibration point for the analyte. It is equivalent to the concentration of the lowest calibration standard, assuming that all Method-specified sample weights, volumes, and cleanup procedures have been employed. According to Method 1668A, laboratories may establish MLs lower than EMLs: MLs may be established as low as the lowest calibration point provided that the concentration of the congener in a minimum of 10 blanks for a sample medium (e.g., water, soil, sludge, tissue) is significantly below the EML. Significant means that the ML for the congener is no less than the average (mean) plus 2 standard deviations above the level in the minimum of 10 blanks. The blanks must be analyzed during the same period that the sample is analyzed, ideally over an approximately 1-month period.

Ongoing Precision and Recovery Standard (OPR) - A method blank spiked with known quantities of analytes. The OPR is analyzed exactly like a sample. Its purpose is to assure that the results produced by the laboratory remain within the limits specified in the method for precision and recovery.

Polychlorinated Biphenyl (PCB) - PCB (or PCBs) is a category, or family, of chemical compounds formed by the addition of chlorine (Cl) to biphenyl ($C_{12}H_{10}$), which is a dual-ring structure comprising two 6-carbon benzene rings linked by a single carbon-carbon bond. The nature of an "aromatic" (benzene) ring allows a single attachment to each

carbon. This means that there are 10 possible positions for chlorine substitution (replacing the hydrogens in the original biphenyl).

A generalized PCB structure showing bonding locations

PCB Congener - Any single, unique, chemical compound in the PCB category is called a "Congener". The name of a congener specifies the total number of chlorine substituents and the position of each chlorine. For example: 4,4'-Dichlorobiphenyl is a congener comprising the biphenyl structure with two chlorine substituents, one on each of the two carbons at the "4" (also called "para") positions of the two rings. There are 209 possible unique PCB congeners.

PCB Homolog - "Homologs" are subcategories of PCBs, representing all congeners having an equal numbers of chlorine substituents. For example, the "Tetrachlorobiphenyls" (or "Tetra-PCBs" or "Tetra-CBs" or just "Tetras") are all PCB congeners with exactly 4 chlorine substituents in any arrangement. The number of congeners in each homolog group are given in the following table:

PCB Homologs			
Homolog	**Abbreviation**	**Cl Substituents**	**PCB Congeners**
Monochlorobiphenyl	MoCB	1	3
Dichlorobiphenyl	DiCB	2	12
Trichlorobiphenyl	TrCB	3	24
Tetrachlorobiphenyl	TeCB	4	42
Pentachlorobiphenyl	PeCB	5	46
Hexachlorobiphenyl	HxCB	6	42
Heptachlorobiphenyl	HpCB	7	24
Octachlorobiphenyl	OcCB	8	12
Nonachlorobiphenyl	NoCB	9	3
Decachlorobiphenyl	DeCB	10	1

PCB Mixture - With few exceptions, PCB was manufactured as a complex mixture of congeners, through progressive chlorination of batches of biphenyl until a certain target percentage of chlorine by weight was achieved. Commercial mixtures with higher percentages of chlorine contained higher proportions of the more heavily chlorinated congeners. While PCB was manufactured and sold under many names, the most common

were the "Aroclor" series (the Monsanto trade name), in many of which a numerical identifier included the percentage of chlorine (e.g., "Aroclor 1254", with 54 percent chlorine).

Preparation blank—See Method blank

Quality assurance (QA) - an integrated system of management activities involving planning, implementation, documentation, assessment, reporting, and quality improvement to ensure that a process, item, or service is of the type and quality needed and expected by the client.

Quality assurance project plan - a formal document describing in comprehensive detail the necessary QA, QC, and other technical activities that must be implemented to ensure that the results of the work performed will satisfy the stated performance criteria.

Quality control (QC) - the overall system of technical activities that measures the attributes and performance of a process, item, or service against defined standards to verify that they meet the stated requirements established by the customer; operational techniques and activities that are used to fulfill requirements for quality.

Quality control check sample (QCS)—A sample containing all or a subset of the analytes at known concentrations. The QCS is obtained from a source external to the laboratory or is prepared from a source of standards different from the source of calibration standards. It is used to check laboratory performance with test materials prepared external to the normal preparation process.

Reagent water—water demonstrated to be free from the analytes of interest and potentially interfering substances at the method detection limit for the analyte.

Relative standard deviation (RSD)—The standard deviation times 100 divided by the mean. Also termed "coefficient of variation."

SPE—Solid-phase extraction; an extraction technique in which an analyte is extracted from an aqueous sample by passage over or through a material capable of reversibly adsorbing the analyte. Also termed liquid-solid extraction.

Signal-to-noise ratio (S/N)—The height of the signal as measured from the mean (average) of the noise to the peak maximum divided by the width of the noise.

Trip Blank - A sample of analyte-free reagent water or other media placed in a sample container in the laboratory and taken from the laboratory to the sampling site and returned to the laboratory unopened. The trip blank is stored and preserved in the same manner as samples and undergoes all sample analytical procedures. A trip blank is used to document potential contamination attributable to shipping and field handling procedures. This type of blank is often used for volatile organics samples.

Unique GC resolution or uniquely resolved—Two adjacent chromatographic peaks in which the height of the valley is less than 40 percent of the height of the shorter peak. This is an indication of the ability of the instrument to separate two or more similar compounds.

VER—See Calibration verification.

Validation - confirmation by examination and provision of objective evidence that the particular requirements for a specific intended use are fulfilled. In design and development, validation concerns the process of examining a product or result to determine conformance to user needs.

Verification - confirmation by examination and provision of objective evidence that specified requirements have been fulfilled. In design and development, verification concerns the process of examining a result of a given activity to determine conformance to the stated requirements for that activity.

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