SEDD SPECIFICATION

and Data Element Dictionary

Version 5.2

For the Staged Electronic Data Deliverable (SEDD)

July 2008

This page intentionally left blank.

Table of Contents

Executive Summary v

1.0 AN OVERVIEW OF SEDD 1

1.1 THE SEDD STAGES 1
1.2 BENEFITS OF SEDD 3
1.3 AN INTRODUCTION TO THE TECHNOLOGY BEHIND SEDD 3

1.3.1 The XML File 3
1.3.2 The Document Type Definition (DTD) 4
1.3.3 Schemas 5

2.0 AN INTRODUCTION TO THE SEDD SPECIFICATION 6

2.1 RELATIONSHIP OF A DTD OR SCHEMA TO THE SEDD SPECIFICATION 6
2.2 THE SEDD SPECIFICATION HIERARCHY 7
2.3 USE OF THE SEDD SPECIFICATION BY THE DATA REQUESTER 8

2.3.1 Common Environmental Analyses (GC, GC/MS, ICP, ICP/MS, CVAA, etc.) 8
2.3.2 Other Types of Analysis 8

3.0 SEDD SPECIFICATION SYNTAX, REQUIRED DATA ELEMENTS, AND DATA ELEMENT VALUE FORMATS 11

3.1 SYNTAX 11

3.1.1 Character and Line Syntax 11
3.1.2 Element Syntax: Data Elements, Names, and Values 13
3.1.3 SEDD Hierarchy, Header and Dependent Data Element Syntax 16
3.1.4 XML File Syntax 18

3.2 TYPES OF REQUIRED DATA ELEMENTS 19

3.2.1 Required Data Elements 22
3.2.2 Conditionally Required Data Elements 22
3.2.3 Data Elements Required for Traceability (Including QC) 22
3.2.4 Data Elements Required for Portability (Including QC) 22

3.3 DATA ELEMENT VALUE FORMATS 23

3.3.1 Text 23
3.3.2 Identifier 23
3.3.3 Limited List 23
3.3.4 Numeric 24
3.3.5 Date 25

4.0 CONCEPTS AND RELATIONSHIPS 26

4.1 Concepts 27

4.1.1 Samples 27
4.1.2 Instrument QC 28
4.1.3 Method 29
4.1.4 Method QC Sample 32
4.1.5 Analysis 32
4.1.6 Results 33

4.2 Relationships 36

4.2.1 Batches 36
4.2.2 Analysis Groups 42
4.2.3 Analyte Groups 46

4.2.4 QC Categories and QC Linkage 47
4.2.5 Comparisons 50

APPENDICES

Appendix A: Data Element Dictionary (DED) A-1

Appendix B: A Visual Representation of the Stages of SEDD (Figures) B-1

Appendix C: Glossary C-1

EXECUTIVE SUMMARY

Purpose

This SEDD Specification document provides the basic knowledge necessary so that laboratories and customers may use the Staged Electronic Data Deliverable (SEDD) to transmit analytical data. This specification provides an overview of SEDD, an introduction to the XML technology behind SEDD, the basic syntax required in order to build a SEDD file, and information regarding the concepts and relationships between the data required to build a hierarchical electronic data deliverable.

About SEDD

The Staged Electronic Data Deliverable (SEDD) is a uniform format for transmitting analytical data. A SEDD file is a text-based document that uses Extensible Markup Language (XML) to store analytical data in an hierarchical manner for transmission between systems. SEDD files may consist of several stages, each successive higher stage including additional analytical data based on the needs of the customer.

Benefits of Using SEDD

The SEDD format provides users with the following benefits:

- a uniform, non-proprietary format to transmit data;
- the ability to perform automated review and validation of data;
- the ability to customize the amount of data reported using the different SEDD stages;
- the ability for data users to define common sets of valid values for methods, analytes, units, etc.;
- cost savings as laboratories automate systems by using SEDD; and
- the ability to generate hardcopy forms and data directly from electronic SEDD files.

This page is intentionally left blank.

1.0 AN OVERVIEW OF SEDD

The Staged Electronic Data Deliverable (SEDD) is a uniform format for the electronic transmission of environmental analytical data. A SEDD file is an Extensible Markup Language (XML) document that can be transmitted and imported into numerous systems and software. The SEDD format, as the name implies, is staged, allowing data requestors to specify what level of detail is reported in their data deliverable, with each successive higher stage providing more data.

1.1 THE SEDD STAGES

The format for SEDD is hierarchical, and is based on a model of laboratory activities, the linkages between these activities, and the data that these activities produce. Data requesters may chose between the following three primary stages of SEDD, based on the level of detail they require.

- **Stage 1** contains the minimum amount of data required to transmit “results-only” data. Only limited method QC data (or no QC data at all) would be reported in Stage 1.

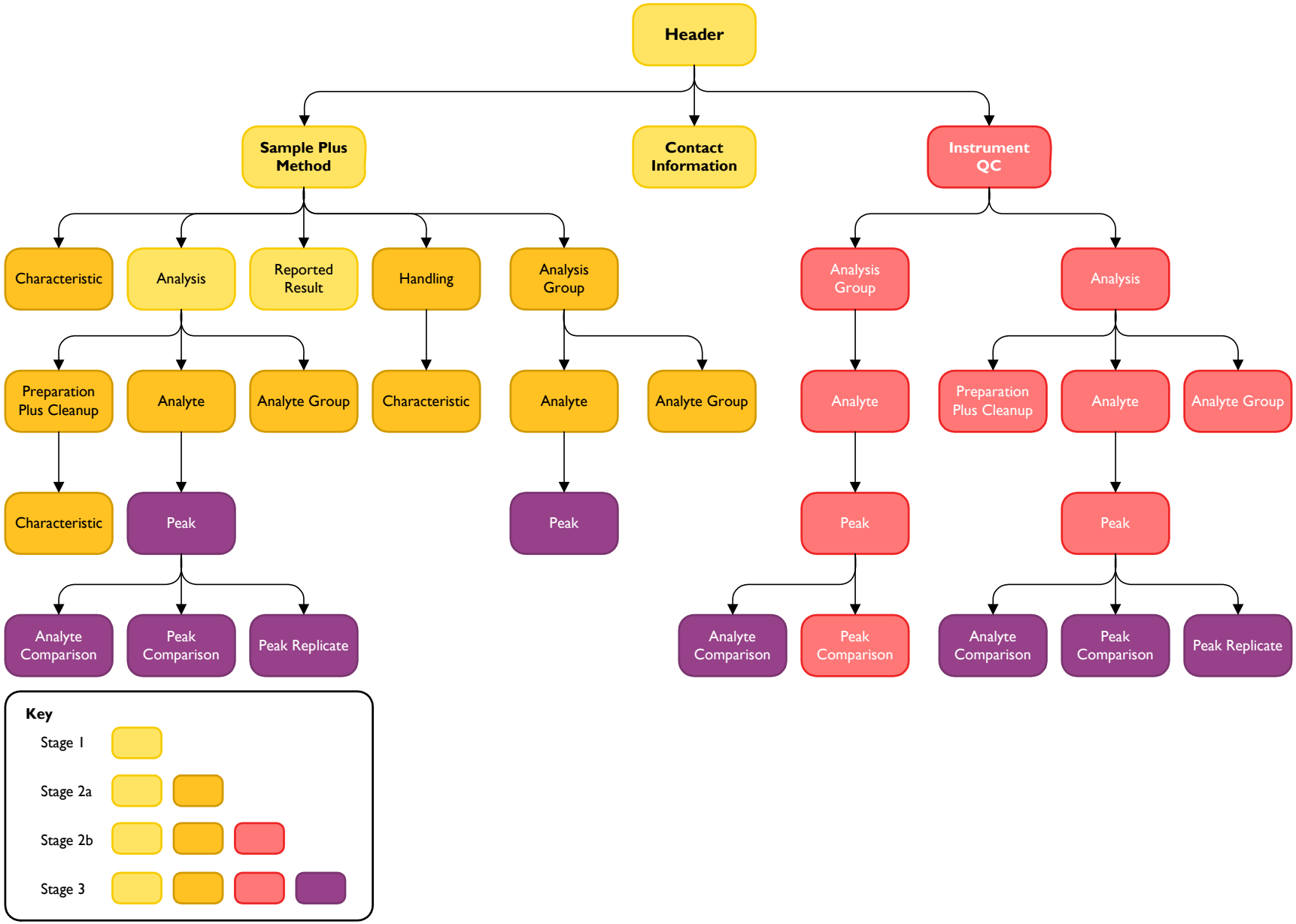
- **Stage 2** has two distinct levels that build on Stage 1. Stage 2a adds method QC data, and Stage 2b adds instrument QC data.

- **Stage 3** builds on stage 2 by adding additional measurement data that allows for independent recalculation of reported results.

- **Stage 4** builds on stage 3 by adding raw instrument data files. This stage has not yet been developed.

Figure 1-1 provides a graphical representation of the additional information that each stage of SEDD provides.

Figure1-1. A Visual Representation of the SEDD Stages



1.2 BENEFITS OF SEDD

The use of SEDD provides benefits to both the data requestor and the data generator. SEDD provides:

- a uniform electronic format for analytical data that can meet the needs of multiple agencies and programs;
- transmittal of data in a non-proprietary XML format, allowing data to be reused by multiple applications and organizations;
- information required to perform automated review and validation of data, with higher levels of validation (even complete recalculation of reported results) available depending on the stage of SEDD chosen;
- the ability for data users to define common sets of valid values for methods, analytes, units, etc.;
- cost savings as laboratories automate the generation of SEDD files directly from Laboratory Information Management Systems (LIMS) or other databases; and
- the ability to generate hardcopy forms and data directly from the electronic SEDD files using XML style sheets.

1.3 AN INTRODUCTION TO THE TECHNOLOGY BEHIND SEDD

NOTE

This section is not intended as a full tutorial on XML. The following information is an overview of the technology used in SEDD and provides some examples to provide the reader with a familiarity with some of the terms and code examples used in this specification. Data requesters and data generators should be familiar with XML to correctly apply the SEDD specification.

1.3.1 The XML File

A SEDD file is an Extensible Markup Language (XML) document. XML is an open standard used to provide a common, flexible way to transfer data over the Web. XML is used for complex document creation and to provide a flexible way to transfer information between databases, users, and organizations. It was developed by the World Wide Web Consortium (W3C) as an extension to Hypertext Markup Language (HTML), commonly used to display documents on the web. XML is not owned by any one vendor and thus remains an open standard. Since XML is text-based, these files may be processed using any platform.

XML files are text-based documents that organize data in a hierarchical manner. XML documents consist of elements, which generally include a start tag describing the piece of data being reported, the data, and an end tag that matches the start tag. For instance,

an element that holds data for a zip code might appear as shown in Example 1-1. Example 1-2 contains an example of what a simple XML document may look like.

Example 1-1. A Data Element

```
<ZipCode>20151</ZipCode>
```

Example 1-2. A Simple XML Document

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE address SYSTEM "address.dtd">
<Address>
   <ContactName>Adam Bryce</ContactName>
   <Street1>9999 Jones Rd.</Street1>
   <Street2>Apt 555</Street2>
   <City>Chantilly</City>
   <State>VA</State>
   <ZipCode>20151</ZipCode>
</Address>
```

Elements may contain data, or can be used to group other elements. Container elements, often called "nodes" (such as "address" in Example 1-1), are used to group similar information, with the container being referred to as a "parent" and the elements it contains being known as "children." If these elements are represented graphically, it results in a tree-like structure. Figure 1-1, which shows the stages of SEDD, is a good example of the tree-like structure that is formed by the many nodes available in a SEDD Document.

1.3.2 The Document Type Definition (DTD)

XML is a powerful and flexible technology that allows for the easy transfer of data. But data users need to ensure that data reaches them in a predictable format that is easily read and manipulated. To be useful to data users, XML files need to be well-formed (have proper XML syntax), and contain the correct data elements in the correct places (have proper XML validation), as expected or dictated by the data user.

A Document Type Definition (DTD) is a document model that dictates all the allowed elements, and describes what kind of elements and data they may contain. DTDs allow data users to

- declare a set of allowed elements that an XML file may contain
- determine which elements or data can go inside an element, the order, the number, and if they are required or not
- set attributes for each element that may be used in the XML document to define a specific setting or provide additional information about the element.

Data users may need to add additional validation checks by using data validation software as produced by a secondary or external company that could be customized to their own data validation needs.

1.3.3 Schemas

Schemas provide a greater level of flexibility and quality control than DTDs. While DTDs provide a large amount of information regarding the structure of an XML file, they have limited impact on the actual content. With schemas, data users can more specifically address the content of an XML file than they could with a DTD. For example, schemas allow data users to specify the data type of each element (string, integer, Boolean, etc). Schemas are more detailed and complex than DTDs, and require an associated level of effort to maintain as the markup language they help define evolves.

2.0 AN INTRODUCTION TO THE SEDD SPECIFICATION

The SEDD (Staged Electronic Data Deliverable) Specification is a set of instructions for developing standardized electronic data deliverable formats for environmental analytical data. SEDD is designed to be Agency and Program neutral. An Electronic Data Deliverable (EDD) is comprised of actual electronic data that is delivered as a unit. The analytical data delivered by laboratories as EDDs to their data requesters includes sample information, laboratory measurements, and Quality Control (QC) information.

The SEDD Specification provides the framework for developing the Document Type Definitions (DTDs) or Schemas and the resultant EDD formats by providing general specifications for the overall data structure of the EDD, while remaining flexible enough to be tailored for present and future individual Program or Agency needs.

The data requester (e.g., Federal or State Agencies, private firms) must first transmit the project requirements to the data generator (e.g., the analytical laboratory). These project requirements would typically include the numbers and types of samples expected for a given project, the specific methods to be used and analytes to be reported, any specific quality control requirements needed along with the associated control ranges and the final data reporting requirements. These reporting requirements would include the specific format (e.g., Document Type Definition or Schema along with any associated valid values) as required for the project. Data is then generated at the analytical laboratory and sent to the data requester in the electronic format required by the data requester. The laboratory would normally be required to check the format and content of the electronic data deliverable using generic tools or tools provided by the data requester to ensure compliance with the data requester's requirements prior to delivery of the data to the data requester. These data are then checked again by the data requester for format and content to ensure the data meets the data requester's contractual and technical requirements and then further processed by combining the data generator's data with other project generated data.

Each data requester must develop a guide based on the SEDD Specification and their individual technical requirements. This guide should include the DTD or eXtensible Markup Language (XML) Schema and a complete set of instructions for developing their specific individual EDD format. For the most common forms of environmental analysis [e.g., Gas Chromatography (GC), GC/Mass Spectrometry (GC/MS), Inductively Coupled Plasma (ICP), and ICP/MS)], DTDs and Schemas have been developed for SEDD and must be used with no modification (see Section 2.3.1).

2.1 RELATIONSHIP OF A DTD OR SCHEMA TO THE SEDD SPECIFICATION

The SEDD Specification provides the requirements for developing DTDs and Schemas and the resultant EDDs for reporting data to meet data requester's (e.g., a Federal Agency) needs. Final DTDs and examples of the resultant EDDs for major environmental methods are available.

The SEDD Specification is flexible in that it can satisfy diverse requirements. The SEDD Specification uses a data model based on analytical activities in an actual laboratory as a starting point for requesting data deliverables. The SEDD Specification uses names for

nodes and data elements to describe typical types of laboratory activities. To take full advantage of the standardization available from the SEDD Specification, data requesters shall use these generalized names in their DTDs or Schemas. A Data Element Dictionary (DED) listing these generalized names is included in Appendix A. A DTD or Schema specifies which of the SEDD Specification nodes and data elements are required.

If, after careful review of the SEDD structure and the SEDD DED, a data requester is convinced that a particular critical requirement of their program is not addressed, specific data elements may be added to the data requester's DTD or Schema to address those needs. The data requester must be aware that implementation of specific data elements particular only to their Program reduce the ability of multiple Programs to share their data. Data requesters must present their specific data element needs to the SEDD Program Manager for possible future incorporation into the SEDD DED that is included within the SEDD Specification (see Section 3.1.2).

A DTD or Schema rarely requires all of the information available in the SEDD Specification. When necessary, a data requester can require additional information. However, all DTDs or Schemas and the resultant EDDs created using the SEDD Specification will use the same structure and DED.

This document, along with the SEDD DED, constitutes the Staged Electronic Data Deliverable (SEDD) Specification for developing the Document Type Definition (DTD) or Schema and the resultant EDD.

This SEDD Specification document is not a comprehensive specification for a specific DTD or Schema and EDD format. Specific DTDs or Schemas and the resultant EDDs must still be fully developed and defined by the data requester using the SEDD specification as a reference. In order to derive the greatest benefits from the XML technology, data requesters must utilize both the SEDD Specification structure and the SEDD Data Element Dictionary.

2.2 THE SEDD SPECIFICATION HIERARCHY

The SEDD Specification hierarchy is based on a model of laboratory activities, the linkages between these activities, and the data these activities produce. To take a typical laboratory scenario, each sample analyzed by one method typically has several results that have to be reported (e.g., a volatile analysis by SW-846 Method 8260 would have many analytes whose concentrations are determined and reported). Information regarding the sample (sample identification) and method (primary analytical method used) would be captured in a SamplePlusMethod node since this information would be the same for all volatile analytes being reported for the sample. One or more analyses may be conducted on this sample by the laboratory. Each analysis performed would be reported as a separate node under the original SamplePlusMethod node. The results of each analysis performed would be captured in Analyte nodes under each Analysis node. The final reportable results for this sample would be reported in ReportedResult nodes. There would be several ReportedResult nodes, one for each of the analytes whose results are being reported, with each of these nodes linked directly to the original SamplePlusMethod node, which represents just part of the overall SEDD structure. The SEDD structure is a three-dimensional hierarchy that is based on this model of laboratory activities.

To take full advantage of the standardization available from the SEDD Specification, data requesters shall use these structures in their DTDs or Schemas. To assist data requesters, the SEDD Specification structure can be implemented in the following three primary stages depending upon the level of detail the data requester needs in the EDD:

- **Stage 1** contains the minimum number of nodes and data elements to transmit "results-only" data. Only limited method QC data (or no QC data) would be reported in Stage 1. The Stage 1 structure is presented in Appendix B, Figure 1.

- **Stage 2** builds on Stage 1 by adding method (Stage 2a) and instrument (Stage 2b) QC data. The Stage 2a structure is presented in Appendix B, Figure 2 and the Stage 2b structure is presented in Appendix B, Figure 3.

- **Stage 3** builds on Stage 2 by adding additional measurement data to allow for the independent recalculation of the reported results. The Stage 3 structure is presented in Appendix B, Figure 4.

- **Stage 4** builds on Stage 3 by adding the actual instrument original raw data files. This Stage has not yet been developed.

2.3 USE OF THE SEDD SPECIFICATION BY THE DATA REQUESTER

2.3.1 Common Environmental Analyses (GC, GC/MS, ICP, ICP/MS, CVAA, etc.)

For the most common forms of environmental analysis, program-neutral DTDs already exist and shall be used to ensure development of a uniform format for the transmission and mutual exchange of environmental analytical data. These DTDs, along with Valid Values for many of the data elements, are provided as separate documents.

Program-specific requirements would be addressed in the instructions to the data generators. These instructions would specify what specific data elements would be required for each method along with any required valid values. These instructions would also address what specific quality control samples would be required along with any specific linkages that would associate these quality control samples to the regular samples. Specific QC acceptance criteria and data-flagging rules would also be specified. It would be highly unlikely that all data elements would be required to be populated for any given program at any given stage. Several examples of these program-specific implementations have been provided as separate documents.

2.3.2 Other Types of Analysis (e.g., Pharmaceutical, Biotechnology, Agriculture, Food and Beverage Testing, etc.)

Use of the SEDD Specification is not restricted to just environmental analysis, but can also be used for any type of chemical, radiological, or microbiological analysis data transfer. To create the DTD or Schema, the data requester must assess the current and future data needs of their program. Data requesters should evaluate which data elements (fields) they currently receive from their laboratories, either in an electronic deliverable or on a hardcopy form. Data requesters should also evaluate the level of assessment they need to apply to the data (e.g., check completeness only, or confirm calculated values). Based on this evaluation, data requesters then select the appropriate

stage from the SEDD Specification. This forms the basis for what nodes and data elements are available.

Based on the specific data items required by the program, the data requester then selects the corresponding data elements from the SEDD DED that are to be populated by the data generator. The data requester would also define which valid values would be appropriate to their program.

In addition to the DTD or Schema, the data requester must also specify the appropriate formats for each element. This would include details on identifying samples, methods, and projects, and specifying the minimum precision for measurements and results and the maximum length of any reported value. The following format considerations must be addressed:

- Define the level of detail required (e.g., Stage 1, Stage 2a, Stage 2b, Stage 3).
- Use the SEDD Specification and define all of the linkages that will be used between the data elements as required by the program.
- Define all valid values associated with the appropriate data elements using the accompanying Valid Value list. Some elements may be restricted to a single valid value while others could have many valid values. For example the data element ResultUnits could have the following valid values associated with it: ug/L, ug/kg, mg/L, mg/kg, etc. A data requester may decide only to allow ug/L for Volatile Organics in a water matrix. Data requesters would be encouraged to allow for flexibility to avoid putting too many specific unique burdens on the data generators.

To assist the data generator in creating the resultant EDD, the data requester will also need to perform the following tasks:

- Make the DTD or Schema and program specifications available to the data generator.
- Work with the data generator to clarify which specific data items already being supplied correspond to which specific SEDD data elements.

Sections 3 and 4 of this Specification present the basic information to create an EDD based on the SEDD specification. Each data requester and data generator must become familiar with the guidelines and requirements given in these two sections. Once they become familiar with the guidelines, specific DTDs or Schemas and special instructions can be created by the data requester. The data generator would use this information to create the EDD.

Section 3 gives the basic rules for presentation of data in each data element, the hierarchy of the elements within the DTD or Schema and the resultant EDD, and the overall EDD file which must meet XML requirements.

Section 4 describes some of the key concepts underlying the SEDD Specification analytical model.

NOTE

Sections 3 and 4 are not meant to be tutorials in XML technology. Only basic XML rules as applicable to the SEDD Specification are summarized. Both the data requester and data generator must be familiar with XML to correctly apply the SEDD Specification.

3.0 SEDD SPECIFICATION SYNTAX, REQUIRED DATA ELEMENTS, AND DATA ELEMENT VALUE FORMATS

This section provides the structural and data representation rules (i.e., syntax) for the SEDD Specification, along with the required data elements, and the format for each data element value. This information is broken into the following three subsections:

- Syntax (see Section 3.1)
- Required Data Elements (see Section 3.2)
- Data Element Value Formats (see Section 3.3)

Data can be transferred between a data generator and a data requester using XML technology only if the specifications regarding the data format have been worked out between the two parties prior to transmission of data (in the form of an XML file). The SEDD Specification provides the basis of the format for transmission of analytical data by clearly defining the overall data structure, data elements, and relationships between the data elements.

NOTE: Most of the examples provided in Sections 3 and 4 pertain to Stages 2a, 2b and 3 of the SEDD Specification. At present, most laboratories deliver EDDs equivalent to Stage 2a of the SEDD Specification (sample results plus method QC data - see Appendix B, Figure 2). Previous experience has demonstrated that most laboratories can implement EDDs based on a Stage 2a SEDD Specification format within a few months. Laboratories can then build on the Stage 2a EDDs to create and deliver Stage 2b (see Appendix B, Figure 3) or Stage 3 (see Appendix B, Figure 4) EDDs by adding additional nodes and data elements to the Stage 2a EDD (as data requestor needs change).

3.1 SYNTAX

Syntax is defined as the rules for representation of data and structure. This section describes the syntax for the following components of SEDD Specification EDDs, as well as the overall file syntax, as follows:

- Characters and Lines (see Section 3.1.1)
- Elements, Names, and Values (see Section 3.1.2)
- SEDD Specification Hierarchy (see Section 3.1.3)
- XML File Syntax (see Section 3.1.4)

3.1.1 Character and Line Syntax

An EDD is a string of characters in a series of lines. The specific character set used would be specified in the opening XML declaration statement to call specific data linkage

library modules/parsers within the operating system program of the computer.

The encoding called UTF-8 (Unicode Transformation Format - 8-bit form) is the default used for SEDD. The UTF-8 character set is backwards compatible with the 128 US-ASCII characters. Expanded versions of UTF-8 can be used along with the use of other character codes sets.

There are five characters that cannot be directly represented in XML. The characters are: &, <, >, “, ‘. These characters must be respectively declared as the following entities: &amp, &lt, &gt, &quot, &apos. However, all current XML parsers and readers convert these entities back to their original characters automatically when the XML document is processed. For example, the value ‘<2’ would appear as ‘&lt2’ in an actual XML document but be correctly rendered as ‘<2’ when the document was processed.

The EDD produced by the SEDD Specification, like all XML documents, is composed of six basic types of lines:

1. **XML declaration line**: This is the first line in an XML document. This first line consists of optional leading spaces; a less than sign followed by a question mark followed by the letters xml; the xml declaration statements; a question mark followed by the greater than sign (e.g., <?xml version="1.0" ?>). The character set used by the EDD would also be specified in this same line (e.g., <?xml version=”1.0" encoding=”UTF-8"?>). The introduction of any others characters at the beginning of this line, as might be introduced by a word processor, could cause the xml file to become unreadable.

2. **Document type declaration lines**: This is the second line in an XML document. This second line consists of optional leading spaces; a less than sign followed by an exclamation mark followed by the letters DOCTYPE; the DOCTYPE declaration statement; followed by the greater than sign (e.g., <!DOCTYPE Header SYSTEM “SEDD_5-2_GENERAL_3_1.dtd”>). This line tells processing software which DTD was used to create the document, providing rules by which it should be processed.

3. **Blank lines**: Contain no characters. Blank lines can occur anywhere in an EDD and are used as white space to provide visual formatting to aid human readers.

4. **Comment lines**: Consist of optional leading spaces; a less than sign, the exclamation mark, two dashes; followed by the comment; followed by two dashes and the greater than sign (e.g., <!-- This is a comment line. -->). A comment line does not need to include the word “comment.”

   Comment lines can occur anywhere in an EDD; however, it is recommended that comments lines not precede XML declaration line or the Document Type declaration line (the typical first two lines in a SEDD EDD file). Their content is not part of the information to be delivered by the EDD. They can be used to annotate an EDD for a browser and might be printed as part of a status report by a program that reads the EDD.

   NOTE: It is important to distinguish a <!-- comment line --> from actual comments made as part of the official EDD itself. Within an EDD, the

Comment data element is used to convey information that may be important for the proper interpretation of the data presented (example: <Comment>This is a comment.</Comment).)

5. **Data element lines**: Consist of optional leading spaces; a less than sign followed by a data element tag name followed by a greater than sign; the data element value; a less than sign followed by the forward slash sign followed by a data element tag name followed by the greater than sign (e.g., <DataElementTag>value</DataElementTag>). A data element usually delivers a single piece of information.

6. **Nodes**: Consist of optional leading spaces; a less than sign followed by a node tag name followed by a greater than sign (e.g., <NodeTag>). A closing node tag name must also be used later in the EDD and consists of optional leading spaces; a less than sign, followed by a forward slash, followed by the same node tag name, followed by the greater than sign (e.g., </NodeTag>). A node contains other data elements.

Using leading spaces to indent lines is a common practice. This technique can be used to group EDD data, improving readability by human readers.

3.1.2 Element Syntax: Data Elements, Names, and Values

Data Elements

A data element tag consists of a start data element tag name followed by the data element value content followed by an end data element tag name (e.g., <Result>24.2</Result>). A data element usually delivers a single piece of information. Data elements are sometimes called fields.

Spaces are not allowed between the start and end tags unless they are an integral part of the data element value.

The SEDD Specification has no rules forbidding the use of any data elements and data requesters cannot add any such rules. If data requesters receive more data elements than originally requested, the data requester should ignore these additional data elements as long as the additional elements are contained in the referenced DTD or Schema.

Definitions for the SEDD Specification data elements are provided in Appendix A.

Data Element Names

A data element name is a string of alphanumeric (A-Z, a-z, 0-9) characters. A name identifies the data delivered by a data element, and should be limited to a maximum of 30 characters.

Character case is significant in names. The first letter of all words used in data element names must be capitalized. Example: AnalyzedDate would be acceptable while Analyzeddate would not.

Implementation-defined names are strongly discouraged but allowed. They must begin with the underscore character (_). A new data element not currently listed in the DED would be named '_NewDataElement.' Useful implementation-defined names will be incorporated in later versions of SEDD under SEDD-assigned names in the SEDD DED. Data requesters are urged to carefully check the SEDD DED to ensure that the needed data element is not already present in the dictionary under another name.

NOTE: Please check with the SEDD Program Manager for any assistance regarding the addition of new data elements.

Names should be spelled-out and each word should have its first letter capitalized (e.g., 'ResultUnits') using the Upper Camel Case (UCC) convention. Excessive abbreviation should be avoided.

Data element names as defined in SEDD are listed in Appendix A with a description of their usage.

Data Element Values

A data element value can contain any string of characters allowed in a line, as restricted by rules defined by the data requester. A value is the data delivered by a data element.

NOTE: Part of the definition of a name is a possible restriction on the format of values associated with it, such as numeric or date formats. Section 3.3 defines these formats.

By SEDD rules, the length of the value is specified by the data requester.

The value begins immediately after the starting data element tag name. In particular, any spaces after this starting tag and before the ending tag are part of the value.

A value can be null (contain no characters). Null values would be reported on a single line using the following format: optional leading spaces; a less than sign, followed by the data element tag name, followed by a forward slash, followed by the greater than sign (e.g., <DataElementTag/>).

Nodes

A node element consists of an opening node tag and a closing node tag which are located on separate lines within the EDD. The opening node tag is a less than sign followed by a node tag name followed by a greater than sign (e.g., <NodeTag>). A closing node tag name must also be used later in the EDD and consists of a less than sign, followed by a forward slash, followed by the same node tag name, followed by the greater than sign (e.g., </NodeTag>).

The first node encountered in the EDD is referred to as the root node. This node can only be used once. All data delivered in the EDD must fall within the opening root node (e.g., <Header>) and the closing root node (e.g., </Header>).

Node Element Names

A node element name is a string of alphanumeric (A-Z, a-z, 0-9) characters, and should be limited to a maximum of 30 characters.

Character case is significant in names. The first letter of all words used in node element names must be capitalized. Example: SamplePlusMethod would be acceptable while SampleplusMethod would not.

The following are the SEDD Specification-defined node element names along with their associated definitions:

Analysis	A parent data element that describes one complete sequence of events, from taking a sample aliquot through the measurement process, as defined as part of one method.
AnalysisGroup	A parent data element that links calculated data associated with multiple analyses for one method.
Analyte	A parent data element that describes the analyte level data from one analysis or one group of analyses.
AnalyteComparison	A parent data element that describes data related to the comparison of two or more analytes such as those data elements that describe the effects of potentially interfering analytes on a peak.
AnalyteGroup	A parent data element that links data associated with multiple measured analytes used to calculate results for another analyte.
Characteristic	A parent data element that identifies and quantifies the intrinsic characteristics associated with a sample as received by a laboratory or after the sample has been processed through a handling or preparation method.
ContactInformation	A parent data element that describes data the name, address and other contact information for the laboratory.
Handling	A parent data element that describes any manipulation of the sample (e.g., filtering, ashing, leaching) prior to taking a sample aliquot for analysis.
Header	A parent data element that describes the format and content of the electronic data deliverable.
InstrumentQC	A parent data element related to instrument or process quality control data (e.g., initial and continuing calibration).
Peak	A parent data element that identifies and reports the actual measurement data related to the analysis of analyte peaks.
PeakComparison	A parent data element that identifies cross-peak comparisons (e.g., abundance ratios, inter-peak resolutions).
PeakReplicate	A parent data element related to multiple peak measurements (e.g., multiple exposure readings).
PreparationPlusCleanup	A parent data element that describes a preparation or

	cleanup process as part of an analysis.
ReportedResult	A parent data element that reports the final reportable results of a method.
SamplePlusMethod	A parent data element that describes one sample analyzed under the criteria of one primary method.

Implementation-defined nodes are not allowed.

Node Elements

A node definition begins at a node definition line and continues until the closing node definition line is encountered.

The contents of a node are the node definition line that starts it, all data elements and other nodes within it, and the node definition line that ends it. In particular, blank and comment lines (<!-- Comments -->, as opposed to Comment data elements) are not part of any node.

Most data element names can only be used in specific nodes (see Appendix A). However, some data element names may appear in more than one node, possibly with slightly different definitions.

A data element name may not appear more than once in any given node.

With the exception of data elements denoted as required by the SEDD specification (see Section 3.2) and those specified as required by a SEDD-compatible EDD implementation, no data element is required to appear in an EDD.

The SEDD specification has no rules restricting the order of data elements in nodes and data requesters cannot add any such rules.

3.1.3 SEDD Hierarchy, Header and Dependent Data Element Syntax

The SEDD specification nodes are arranged in a hierarchy. Figure 4 (see Appendix B) defines this hierarchy. As implied by the term hierarchy, nodes at any level can repeat as many times as needed.

Subject to the rules associated with the hierarchy, there are no restrictions on the number, type, and order of nodes in an EDD and a data requester cannot add any. For example, an empty EDD is valid, if not useful. Data requesters can choose to ignore nodes they do not recognize or which are of no interest to them.

Parent nodes with identical content cannot be repeated. For example, a SamplePlusMethod node could not be repeated before each individual ReportedResult node associated with it. It is more efficient to only have one SamplePlusMethod node for all associated ReportedResults' nodes.

NOTE: Data requesters need to check an EDD for global consistency of all potentially redundant data.

Header Nodes

A Header node is always the first node in an EDD. It provides the information (e.g., EDD version and implementation identification) needed to identify and process the EDD reliably.

Each Header node can only refer to and report data based on a single DTD or Schema. Data for a single method or multiple methods can be reported under a single Header node provided that the same DTD or Schema can be used by each method. The choice of how data is to be reported should be conveyed to the data generator from the data requester.

Data processing must start fresh at each new Header node encountered.

Other Nodes

In an EDD, all other nodes must be preceded by at least one node at each higher level. Figure 4 (see Appendix B) defines the dependencies between these nodes. For example, the SamplePlusMethod node is dependent on a Header node.

Any given node is said to be associated with the closest preceding node at each higher level in an EDD.

The pattern of associated higher-level nodes must match the same pattern as in Figure 4 (see Appendix B). For example, in order to have a valid ReportedResult node in an EDD, it must be preceded by a SamplePlusMethod node and a Header node, as shown in Figure 4 (see Appendix B). There cannot be an InstrumentQC node between the ReportedResult and SamplePlusMethod nodes. Otherwise, the ReportedResult node would not properly relate to the sample it should be associated with. This concept is called nesting. All nodes must be properly nested.

When more than one node of a higher level and identical type precedes another node, the dependent node is related to the nearest higher order node as shown in Example 3-1 (comment lines are used to explain the hierarchy).

Example 3-1.

```
<!-- Header Node - Beginning Tag -->
<Header>
   <!-- First SamplePlusMethod Node - Beginning Tag -->
   <SamplePlusMethod>
      <!-- First Result associated with first SamplePlusMethod node -
->
      <ReportedResult></ReportedResult>
      <!-- Second Result associated with first SamplePlusMethod node
-->
      <ReportedResult></ReportedResult>
      <!-- First SamplePlusMethod node - Ending Tag -->
   </SamplePlusMethod>

      <!-- Second SamplePlusMethod node - Beginning Tag -->
   <SamplePlusMethod>
```

```
      <!-- First Result associated with second SamplePlusMethod node
-->
      <ReportedResult></ReportedResult>
      <!-- Second Result associated with second SamplePlusMethod node
-->
      <ReportedResult></ReportedResult>
   <!-- Second SamplePlusMethod node - Ending Tag -->
   </SamplePlusMethod>
   <!--  Header  node - Ending Tag -->
</Header>
```

While the order of nodes at different levels is important in the EDD, the order of nodes at the same level is not. This is shown in examples 3-2 and 3-3, where the ReportedResult and Analysis Nodes are at the same level. These two examples are identical in meaning, but differ in order. All of the ReportedResult nodes in both examples associate, hierarchically, to the preceding SamplePlusMethod node. The Analysis node in each example also belongs, hierarchically, to the same SamplePlusMethod node. The Analysis node does not modify any of the ReportedResult nodes in the second example, even though it precedes it. This is because the Analysis node is not of a higher level than the ReportedResult node.

Example 3-2.

```
<Header>
   <SamplePlusMethod>
      <ReportedResult></ReportedResult>
      <ReportedResult></ReportedResult>
      <ReportedResult></ReportedResult>
      <Analysis></Analysis>
   </SamplePlusMethod>
</Header>
```

Example 3-3.

```
<Header>
   <SamplePlusMethod>
      <ReportedResult></ReportedResult>
      <Analysis></Analysis>
      <ReportedResult></ReportedResult>
      <ReportedResult></ReportedResult>
   </SamplePlusMethod>
</Header>
```

3.1.4 XML File Syntax

Data will be delivered from data generators to their data requesters as XML documents. These XML documents will be both well-formed and valid data files.

A well-formed XML document follows all of the official XML rules as defined by the World Wide Web Consortium (W3C). Many of these rules have already been discussed in previous sections. Data requesters are encouraged to acquaint themselves further with XML using some of the many resources available at this time. A well-formed XML document will have all of its data elements properly nested.

A valid XML document is a document that follows the DTD file or XML Schema as

established by the data requester. The DTD or XML Schema gives the hierarchical structure and states what data elements will be applicable for a given application. A valid XML document can contain fewer data elements than its associated DTD or Schema but cannot contain additional data elements that are not defined by the DTD or Schema even though they may appear in the SEDD Data Element Dictionary.

3.2 TYPES OF REQUIRED DATA ELEMENTS

A few data elements are required to have non-null values to properly and uniquely identify the reported data. If a node is not required, any data element it may contain is not required. The SEDD Specification has four types of required data elements:

- Required Data Elements (see Section 3.2.1)
- Conditionally Required Data Elements (see Section 3.2.2)
- Data Elements Required for Traceability (see Section 3.2.3)
- Data Elements Required for Portability (see Section 3.2.4)

The Data Element Dictionary (Appendix A) gives the type for each data element.

Below is a useful summary of these required data elements per node. Each data element is listed with a code that identifies it as a: (1) Required data element; (2) Conditionally Required data element; (3) Required for Traceability data element; (4) Required for Portability data element.

Header Node

EDDID (1)
EDDImplementationID (1)
EDDImplementationVersion (1)
EDDVersion (1)
LabID (1)

Analysis Node

AnalysisGroupID (2)
AnalysisType (1)
ClientMethodID (1)
LabAnalysisID (1)
LabID (1)
LabMethodID (3)
MethodID (4)
MethodSource (4)
MethodVersion (4)
OriginalLabAnalysisID (2)

AnalysisGroup Node

AnalysisGroupID (2)
AnalysisType (1)

Analyte Node
AnalyteGroupID (2)
AnalyteName (4)
AnalyteNameContext (4)
AnalyteType (1)
CASRegistryNumber (4)
ClientAnalyteID (1)
LabAnalyteID (3)
PeakID (2)
ResultType (1)

AnalyteComparison Node
AnalyteName (4)
AnalyteNameContext (4)
CASRegistryNumber (4)
ClientAnalyteID (1)
LabAnalyteID (3)

Characteristic Node
CharacteristicType (2)

AnalyteGroup Node
AnalyteGroupID (2)
AnalyteName (4)
AnalyteNameContext (4)
AnalyteType (1)
CASRegistryNumnber (4)
ClientAnalyteID (1)
LabAnalyteID (3)
ResultType (1)

ContactInformation Node
LabID (1)

Handling Node
ClientMethodID (1)
LabID (1)
LabMethodID (3)
MethodID (4)
MethodSource (4)
MethodVersion (4)

InstrumenyQC Node
ClientMethodID (1)
LabID (1)
LabInstrumentQCID (2)
LabMethodID (3)
MethodID (4)
MethodSource (4)
MethodVersion (4)

QCLinkage (4)
QCType (1)

Peak Node
PeakID (2)
ResultType (1)

PeakComparison Node
AnalyteName (4)
AnalyteNameContext (4)
CASRegistryNumber (4)
ClientAnalyteID (1)
LabAnalyteID (3)
PeakID (2)

PeakReplicate Node
PeakReplicateID (2)
ResultType (1)

PreparationPlusCleanup Node
ClientMethodID (1)
LabID (1)
LabMethodID (3)
MethodID (4)
MethodSource (4)
MethodVersion (4)

ReportedResult
AnalysisGroupID (2)
AnalyteGroupID (2)
AnalyteName (4)
AnalyteNameContext (4)
AnalyteType (1)
CASRegistryNumber (4)
ClientAnalyteID (1)
LabAnalysisID (1)
LabAnalyteID (3)
PeakID (2)
ResultType (1)

SamplePlusMethod Node
ClientMethodID (1)
ClientSampleID (1)
LabID (1)
LabMethodID (3)
LabSampleID (3)
MatrixID (1)
MatrixMedium (4)
MethodID (4)
MethodSource (4)

MethodVersion (4)
OriginalClientSampleID (2)
OriginalLabSampleID (2)
QCCategory (4)
QCLinkage (4)
QCType (1)

3.2.1 Required Data Elements

Required data elements are the basis for reliable identification of EDD data by the data requestor. Examples include QCType, AnalysisType, and AnalyteType. These data elements MUST be present in a valid EDD.

3.2.2 Conditionally Required Data Elements

Conditionally required data elements also are the basis for identification and linkage of data, but are not required in all cases. Examples include OriginalClientSampleID, required for certain QC samples; LabInstrumentQCID, required when reporting Instrument QC samples; and AnalysisGroupID, required when multiple analyses are used to generate a single result. Based on rules specified for each data element in Appendix A, these data elements must be present in a valid EDD.

3.2.3 Data Elements Required for Traceability (Including QC)

The SEDD Specification has standard data elements to use when traceability back into the laboratory's process is desired. Examples include LabSampleID and LabAnalyteID. These data elements are not formally required by the SEDD Specification, but are suggested as likely to be required in the instructions from the data requester to the data generator.

3.2.4 Data Elements Required for Portability (Including QC)

The SEDD Specification has standard data elements to use when portability of data across sites and/or data requesters is desired. Examples include AnalyteName, QCCategory, and QCLinkage. These data elements are not required by the SEDD Specification, but are suggested as likely to be required in the instructions from the data requester to the data generator.

The SEDD Specification requires the use of all required and conditionally required, as applicable, data elements. Data requesters may require additional data elements based on program needs.

For consistency, the SEDD Specification has required data elements in many nodes that serve to uniquely identify the data. For example, the PeakID data element in a Peak node is a conditionally required data element. It is needed to uniquely identify a peak in a GC/MS analysis. A reasonable value for the PeakID data element is the mass of the peak being used for quantitation.

There are some situations where no unique values exist for the required data element. For example, the ClientAnalyteID data element in a ReportedResult node is a required

data element. However, there would be no real ClientAnalyteID for a Tentatively Identified Compound (TIC) as might be reported during a GC/MS analysis. In this situation the data requester must define how this data element will be used for TICs (i.e., ClientAnalyteID = Unknown_Hydrocarbon01).

As noted in the beginning of this section, the data requester must specify the values for these required data elements if SEDD required valid values are not available.

3.3 DATA ELEMENT VALUE FORMATS

There are five different types of data that can be entered into a given data element. These five types are the data element value formats. These formats are Text, Identifier, Limited List, Numeric, and Date. The Data Element Dictionary (Appendix A) gives the format for each data element.

The examples given below are a partial list of the most commonly used formats. The data requester must specify the exact format of each data element depending on program needs.

3.3.1 Text

Text format allows any value consistent with the syntax of a line. Case is significant in Text format so that “Test” and “TEST” are different values for a Text data element. If data is to be parsed to a database, this may be less of an issue.

Leading and trailing spaces are significant in Text data element values.

3.3.2 Identifier

Identifier format is a restricted version of Text format. Typically, these values use a restricted character set. The data requester should provide instructions for each data element with this format.

A suggestion is that characters be restricted to alphabetic characters, digits, the underscore character, and the dash character and that case not be treated as significant. Identifiers can have further restrictions, such as check digits in CAS Numbers or certain required patterns of alphabetic and numeric characters.

3.3.3 Limited List

Limited list format is another restricted version of Text format. Typically, these values are limited to a short list of valid values. The DTD or Schema could specify the program-specific valid values for each data element with this format. However, in most cases, these valid values are supplied by the data requester and would typically be a subset of the more global valid value lists. Valid values may depend on the value of other data elements. For example, valid values for the ResultUnits data element would typically depend on the MatrixID data element.

3.3.4 Numeric

Numeric format includes any of the following formats:

- **Integer**: leading spaces, a minus sign, a string of digits and trailing spaces, with all subparts optional. The value is interpreted as a whole number.

- **Decimal**: leading spaces, a minus sign, a string of digits, a decimal point, another string of digits and trailing spaces, with all parts but the decimal point optional. The value is interpreted as a real number.

- **Exponential**: leading spaces, a minus sign, a string of digits, a decimal point, another string of digits, a string of spaces, the letter “E” or “e”, a string of spaces, a plus or minus sign, a string of digits and trailing spaces.

A data requester should be prepared to accept any of the possible numeric formats. A data requester must be prepared to read all three formats within the same data stream. However the data requester can specify rules for this format.

Please note the following items regarding the use of a numeric format in an EDD:

- The same number can be expressed in an EDD in the following ways and all are allowable:

12345	Integer format
12345.000	Decimal format
12345E 0	Exponential format with a zero exponent

  If any of the above values are preceded by a minus sign, they are valid numbers.

- Legal values for zero include, but are not limited to:

  0
  0.0
  0.0e0

The SEDD Specification by itself does not limit the precision of numbers. Data requesters should specify minimum acceptable significant digits and/or precision for every numeric data element used. However, it is recommended that all raw data be reported to the full significance as supplied by the instrument.

The SEDD Specification does not specify rounding rules. This has to be specified by the data requester. However, it is recommended if rounding rules are specified by the data requester, that these rules apply only to values that will be reported as final values and will not be used in any subsequent calculations.

A null value for a numeric data element represents a totally blank value, which is not considered equivalent to the number zero. For example, reporting a zero value for a non-detected analyte would not be appropriate since for some methods, zero could be considered an actual measured and valid value itself.

3.3.5 Date

The default date format is (based on ISO 8601:2004):

YYYY-MM-DDThh:mm:ss.sTZD

Where:

YYYY	=	four digit year
MM	=	two digit month (01 = January, etc.)
DD	=	two digit day of month (01 through 31)
T	=	character separator between the date and time
hh	=	two digits of hour (00 through 23) (am/pm not allowed)
mm	=	two digits of minute (00 through 59)
ss	=	two digits of second (00 through 23)
s	=	one or more digits representing a decimal fraction of second
TZD	=	time zone designator (Z or +hh.mm or -hh.mm)

The time zone designator and time portion of a date is optional unless required by a data requester for specific data elements. The seconds portion of the time, with any colon, is similarly optional.

All date format values in the data stream following a Header parent data element must be in the same date format. This format is specified by the DateFormat data element in the Header node (see Appendix A).

NOTE: Other date formats can be used as specified in Appendix A.

4.0 CONCEPTS AND RELATIONSHIPS

Methods used for the analysis of environmental samples are complicated procedures that include sample preparation (digestion or extraction), cleanup of sample extracts prior to analysis, and the actual instrumental analysis. There are many associations for a single sample analysis that must be captured in a unique way if the whole process has to be reconstructed. This is especially important if the data requester wants to clearly link all Quality Control (QC) data with the sample result.

Describing associations among data elements is essential for an EDD to be useful. Because of the variety of batches, groupings, linkages, and comparisons needed for each data requester, specifying a DTD or Schema and the resultant EDD that correctly describes a method can be difficult. Section 4.1 describes some of the main concepts underlying the SEDD Specification, as follows:

- Samples (see Section 4.1.1)
- Instrument QC (see Section 4.1.2)
- Method (see Section 4.1.3)
- Method QC Sample (see Section 4.1.4)
- Analysis (see Section 4.1.5)
- Results (see Section 4.1.6)

Section 4.2 provides a discussion of the more complicated analytical relationships within the SEDD Specification. Batches typically involve linking the Method Quality Control samples (e.g., Laboratory Control Samples, Method Blanks, Matrix Spikes) analyzed to the regular field samples. Analysis Groups (under the SamplePlusMethod node) are used whenever the final reported result for a field sample is computed from more than one separate analysis result as in the case of Method of Standard Additions for Inorganic Analysis. Analysis Groups (under the InstrumentQC node) are used whenever multi-point initial calibration curves are determined. QC Linkages specify which batch types are used to link QC samples to regular field samples. Comparisons are used to relate individual measurements to other reference measurements for Quality Control purposes. The remainder of Section 4 is divided into the following sections:

- Batches (see Section 4.2.1)
- Analysis Groups (see Section 4.2.2)
- Analyte Groups (see Section 4.2.3)
- QC Categories and QC Linkages (see Section 4.2.4)
- Comparisons - Peak and Analyte (see Section 4.2.5)

This section makes liberal use of examples drawn from actual EDDs developed under this specification. Examples in this section have been formatted to aid readability. Formatting conventions need not be adopted when preparing an EDD. While reviewing the following concepts and analytical relationships, Figure 4 (see Appendix B) will be a useful reference for the hierarchy of the nodes in the SEDD Specification.

4.1 Concepts

The fundamental concepts within the SEDD Specification include various types of samples likely to be encountered, the methods used for their analysis, and the reporting of results.

4.1.1 Samples

A sample is defined in the SEDD Specification as any substance given a sample number or identifier. This includes ones sent by a data requester to the data generator (e.g., an analytical laboratory) for analysis and certain Method QC samples (e.g., Laboratory Control Samples (LCSs), Method Blanks) generated by the data generator (see Section 4.1.4). In a SEDD Specification-compatible EDD, each unique sample is reported in SamplePlusMethod and related nodes (i.e., all nodes located below the SamplePlusMethod node in the hierarchy) based on the application of one primary analysis method (see Appendix B, Figure 4).

NOTE: The SEDD Specification does not have a per-sample node. This is because the notion of what a “sample” is as reported in an EDD is ambiguous. For example, the sample might be what is identified by the following data elements within the SamplePlusMethod node: ClientSampleID, FieldSampleID, or LabSampleID. In real cases involving multiple methods, handlings, and reanalyses, these data elements may have different values.

The SEDD Specification uses the SamplePlusMethod node as its highest-level of reporting for samples. The association between the method and a sample must be clear to both the data requester and the data generator. This association is NOT necessarily provided as part of the DTD or Schema and must be provided by the data requester in their instructions to the data generator.

<u>Example Sample Definition</u>

Some programs may report a dilution of an original sample as a separate sample (i.e., using two separate SamplePlusMethod nodes) with a distinct ClientSampleID data element and a separate set of results in each SamplePlusMethod node. When a program reports a dilution of a sample separately from its original in a SEDD Specification-compatible implementation, then two separate SamplePlusMethod nodes will be used, one node to report the complete results of the original sample and the second node to report the complete results of the diluted sample. For this definition, the data requester must provide the data generator with clear instructions as to how to uniquely identify each sample. In contrast, other programs may consider dilutions to be internal to the methods and only report one set of complete ‘best’ results in the one SamplePlusMethod node. This latter approach is the one most often encountered. However, it is important that the data requester convey the approach to be used to the

data generator. Regardless of the approach used, both approaches can deliver the same amount of data from the data generator to the data requester.

The following information must also be defined in the data requester instructions to ensure the uniqueness of each SamplePlusMethod node within the EDD:

- In each SamplePlusMethod node, a sample should have a well-defined matrix identified by the MatrixID data element.
- In each SamplePlusMethod node, the primary analytical method applied is identified by a ClientMethodID and possibly a MethodID and LabMethodID data elements.
- In each SamplePlusMethod node, the type of the sample being analyzed is identified by the QCType data element. Here is where a regular sample would be differentiated from a QC or other type of sample.

Example 4-1, derived from the SW-846 Semivolatile data for Method 8270, illustrates how the various activities in one method are reported in XML format. This example only uses the SamplePlusMethod node. In this example, the primary method applied to the sample, as identified by the ClientSampleID data element, is identified by the ClientMethodID data element. The MatrixID, LabSampleID and QCType data elements are used in conjunction with the ClientSampleID and ClientMethodID data elements to uniquely identify this sample.

Example 4-1.

```
<SamplePlusMethod>
   <ClientMethodID>8270C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <CollectedDate>2007-12-03</CollectedDate>
   <MatrixID>Water</MatrixID>
   <LabReceiptDate>2007-12-04</LabReceiptDate>
   <LabSampleID>M071204-004</LabSampleID>
   <QCType>Field_Sample</QCType>
</SamplePlusMethod>
```

4.1.2 Instrument QC

Any analysis not reportable as part of the data for a sample (as defined in Section 4.1.1) is generically called instrument QC and is reported in InstrumentQC and related nodes (all nodes located below the InstrumentQC node in the hierarchy - see Appendix B, Figure 4).

One InstrumentQC node conveys information associated with one QC measurement, classified by a QCType data element (e.g., calibrations, instrument blanks). Analyses not directly associated with the primary analytical instrument (e.g., GPC calibrations) are also included.

Typically, only one analysis is reported under one InstrumentQC node. However, some types of instrument QC require multiple analyses to assess a particular performance characteristic. For example, many initial calibrations require multiple analyses to assess

linearity of instrument response. In this case, multiple analyses are reported under one InstrumentQC node, using AnalysisGroup nodes to report values computed from the multiple analyses. Each InstrumentQC node must be uniquely identified through the use of the LabInstrumentQCID data element.

Example 4-2, derived from the SW-846 Semivolatile data for Method 8270, illustrates how the various InstrumentQC activities in one method are reported in XML format. This example only uses the InstrumentQC node. In this example, the primary method applied to the InstrumentQC sample is identified by the ClientMethodID data element. The LabInstrumentQCID and QCType data elements are used in conjunction with the ClientMethodID data element to uniquely identify this InstrumentQC sample.

Example 4-2.

```
<InstrumentQC>
   <ClientMethodID>8270C</ClientMethodID>
   <LabInstrumentQCID>CCV-01</LabInstrumentQCID>
   <QCType>Continuing_Calibration_Verification</QCType>
</InstrumentQC>
```

4.1.3 Method

A method corresponds to a defined process for the identification and quantitation of selected analytes. The analyte list for a method often corresponds to compounds or substances measurable after one analysis on one analytical instrument.

A method should include specifications for the type, frequency, and performance criteria for QC samples.

Details of a method can be client-specific. The following SEDD Specification data elements, ClientID, ClientMethodID (for the instrumental analysis), and MatrixID, are used to identify, not describe, a method. This allows the reader of an EDD to look up in their own database whatever method characteristics are needed to correctly process the data. Some programs, such as the Contract Laboratory Program (CLP), define the method to include all of the sample processing steps. Other programs, such as SW-846, will define unique methods for each of these steps.

The SEDD Specification defines four types of activities or measurements associated with applying a method to a sample: characteristic; handling; preparation; and analysis.

<u>Characteristic</u>

Characteristic applies to the sample as received by the data generator. This includes recording or measuring sample characteristics such as color, texture, temperature, moisture, pH, etc. All such data is reported in Characteristic nodes under the appropriate SamplePlusMethod node using various data elements.

In some cases, a characteristic such as Percent Moisture can be reported in one of two possible ways. The first, and most common approach is to treat Percent Moisture as a characteristic property of the sample itself and report it using only the CharacteristicType, CharacteristicValue and CharacteristicUnits data elements in the Characteristic node under the associated SamplePlusMethod node. In addition to the

approach described above, the Percent Moisture could be treated and reported as a separate test entirely. For this situation, this test would then be reported in a separate SamplePlusMethod node with a separate ReportedResult node for Percent Moisture.

Characteristic can also apply to the samples that have been processed through a handling procedure or after going through a preparation or cleanup process. In this case, the characteristic would be the measured property after completion of the identified process.

Handling

Handling applies to any manipulation of the sample prior to taking an aliquot for preparation/analysis. Examples include filtering, decanting, drying, grinding, ashing, and leaching [Toxicity Characteristic Leaching Procedure (TCLP) in particular]. All such data is reported in a Handling node under the associated SamplePlusMethod node. Each Handling node is identified by a ClientMethodID or HandlingType data element. If a handling process is performed, the aliquot taken for analysis is taken from the material as generated from the handling process rather than from the original sample as received by the laboratory.

Many methods have no handling processes associated with them and no Handling node is required in these cases. Occasionally, more than one handling is done, so more than one Handling node is required.

Characteristics of the sample generated after the handling process are captured in Characteristic nodes located under the Handling node.

Preparation and Cleanup

Preparation and Cleanup applies to all processing done to an aliquot prior to analysis. The details might involve many steps (e.g., taking an aliquot, extraction, and cleanup). Most methods have a primary processing step, such as chemical extraction or separation that are part of the analysis method. These steps could also be described in a separate method(s). The specific preparation and cleanup details would normally be captured in a separate PreparationPlusCleanup node, not in the Analysis node.

For analyses that require a minimum or no preparative and/or cleanup steps, no PreparationPlusCleanup node(s) would be needed.

PreparationPlusCleanup nodes are used to report specific preparation steps, especially when a separate method is used to describe this activity. These are similar to Handling nodes in that there might be none, one, or several, depending on the method. The difference is that a PreparationPlusCleanup node applies to one aliquot used in a preparation, while a Handling node applies to one sample prior to taking an aliquot. The ClientMethodID or PreparationType data element in the PreparationPlusCleanup node is used to characterize the preparation event.

The ClientMethodID or CleanupType data element in the PreparationPlusCleanup node is used to characterize the preparation and/or cleanup event.

The PreparationPlusCleanupType data element is used to identify the process as either

a preparation or cleanup event.

Characteristics of the extracted or cleaned up sample after the PreparationPlusCleanup process are captured in Characteristic nodes located under the PreparationPlusCleanup node.

Analysis

Instrumental analysis, also called the determinative step, is where measurements are made for a list of analytes. Values such as instrument identification and date analyzed are reported in the Analysis node. Analyte-specific values from this analysis are reported in Analyte nodes under the Analysis node.

If the analytical technique involves measurements of multiple peaks per analyte [e.g., Gas Chromatography (GC)/Mass Spectrometry (MS) mass spectra, multi-component GC analytes, Inductively Coupled Plasma (ICP) emission spectra], details would normally be reported in Peak nodes under each Analyte.

Example 4-3, derived from the SW-846 Semivolatile data for Method 8270, illustrates how the various activities in one method are reported in XML format. This example uses the following Nodes: SamplePlusMethod; Characteristic; Analysis; and PreparationPlusCleanup. The Analyte node is not used. For the single sample being reported, two characteristics (Temperature and pH) are being reported in two Characteristic nodes. A single analysis is being performed on the sample. Two PreparationPlusCleanup nodes are used, one to report the details of the actual aliquoting and extraction of the sample and the second to report the details of a cleanup step that was conducted on the prepared extract. Notice that according to the dates reported, that the sample was first extracted, then cleaned up, then analyzed.

Example 4-3.

```
<SamplePlusMethod>
   <ClientMethodID>8270C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <CollectedDate>2007-12-03</CollectedDate>
   <MatrixID>Water</MatrixID>
   <LabReceiptDate>2007-12-04</LabReceiptDate>
   <LabSampleID>M071204-004</LabSampleID>
   <QCType>Field_Sample</QCType>

   <!-- typical characteristics -->

   <Characteristic>
      <CharacteristicType>Temperature</CharacteristicType>
      <CharacteristicValue>4.4</CharacteristicValue>
      <CharacteristicValueUnits>C</CharacteristicValueUnits>
   </Characteristic>
   <Characteristic>
      <CharacteristicType>pH</CharacteristicType>
      <CharacteristicValue>6</CharacteristicValue>
      <CharacteristicValueUnits></CharacteristicValueUnits>
   </Characteristic>

   <!-- instrumental analysis -->
```

```
   <Analysis>
      <LabAnalysisID>SV422</LabAnalysisID>
      <ClientMethodID>8270C</ClientMethodID>
      <AnalyzedDate>2007-12-24T14:38</AnalyzedDate>
      <DilutionFactor>1</DilutionFactor>
      <ResultBasis>Total</ResultBasis>

      <!-- a typical preparation -->

      <PreparationPlusCleanup>
         <PreparationPlusCleanupType>Preparation
         </PreparationPlusCleanupType>
         <ClientMethodID>3520B</ClientMethodID>
         <AliquotAmount>1.00</AliquotAmount>
         <AliquotAmountUnits>L</AliquotAmountUnits>
         <FinalAmount>1.00</FinalAmount>
         <FinalAmountUnits>mL</FinalAmountUnits>
         <PreparedDate>2007-12-07T08:30</PreparedDate>
      </PreparationPlusCleanup>

      <!-- a typical cleanup event -->

      <PreparationPlusCleanup>
         <PreparationPlusCleanupType>Cleanup
         </PreparationPlusCleanupType>
         <ClientMethodID>3640A</ClientMethodID>
         <CleanedUpDate>2007-12-08T11:00</CleanedUpDate>
         <InitialAmount>1.00</InitialAmount>
         <InitialAmountUnits>mL</InitialAmountUnits>
         <FinalAmount>1.00</FinalAmount>
         <FinalAmountUnits>mL</FinalAmountUnits>
      </PreparationPlusCleanup>

   </Analysis>
</SamplePlusMethod>
```

4.1.4 Method QC Sample

A QC sample suitable for reporting in SamplePlusMethod nodes is called a method QC sample (e.g., Laboratory Control Sample, Method Blank, Matrix Spike). Its matrix should be well defined. Results are normally reported in the same units as the associated regular samples. Method QC samples are a component of performance-based evaluation of analytical data.

No handling may be associated with Method QC samples. However, they are prepared in the same manner as regular samples.

4.1.5 Analysis

The SEDD Specification defines an analysis as one complete sequence of events starting with an aliquot or prepared sample, perhaps involving preparation, and including an instrumental analysis. This information would be captured in the Analysis node and related nodes (all nodes located below the Analyses node in the hierarchy - see Appendix B, Figure 4). An analysis may be part of a method applied to a sample or part

of an instrumental QC process. Thus Analysis nodes are present under both the SamplePlusMethod node and the InstrumentQC node.

4.1.6 Results

The final results of a method are always reported in ReportedResult nodes. Final results that are associated with a specific analysis can also be reported in Analyte nodes. These final results take into consideration any dilutions or Percent Moisture calculations that would be needed to compute the final results.

> **NOTE:** In the simple case of only one analysis per method, the same values could be reported in both ReportedResult and Analyte nodes. The ReportedResult nodes are required. The Analyte nodes are optional and might be used to report final measurements from multiple analyses or from both a primary and confirmation analyses.

The SEDD Specification distinguishes between the result of a method (e.g., reported concentration of benzene of 250 ug/L in a groundwater sample by Method 8260) and the result of an analysis. Method results are reported in ReportedResult nodes directly under the SamplePlusMethod node. Analysis results can be reported in Analyte nodes under Analysis nodes.

Because InstrumentQC does not have a method-like result, no ReportedResult nodes are used.

Certain analytes in certain methods are always measured on a per-analysis, not per-method, basis (e.g., surrogates and internal standards). These analytes should be reported in Analyte nodes only, not in ReportedResult nodes. For example, in the analysis of pesticides, there are separate surrogate recoveries computed for each column used for a typical primary and secondary column analysis and the surrogate analyte results must be reported in Analyte nodes under each respective analysis.

Each ReportedResult can be linked to its underlying supporting data in one of three possible ways:

1. The data element LabAnalysisID is used to link a ReportedResult to a SINGLE underlying Analysis that was used to produce that result. The LabAnalysisID data element must be present in both the ReportedResult node and in the associated Analysis node and populated with the same value.

2. The data element AnalysisGroupID is used to link a ReportedResult to MULTIPLE underlying Analyses that were used to produce and compute that result. The AnalysisGroupID data element must be present in the ReportedResult node and in the associated Analysis nodes and also present in a separate AnalysisGroup node. See Section 4.2.2 for a complete discussion of analysis groups. In this case, the LabAnalysisID and AnalyteGroupID data elements would not be used.

3. The data element AnalyteGroupID is used to link a ReportedResult to MULTIPLE measured analytes that were used to produce and compute that result. The

AnalyteGroupID data element must be present in the ReportedResult node and in the associated Analyte nodes and also present in a separate AnalyteGroup node. In this case, the LabAnalysisID and AnalysisGroupID data elements would not be used. See Section 4.2.3 for a complete discussion of analyte groups. For each analyte reported as a final result of a method, either the LabAnalysisID, AnalysisGroupID or AnalyteID must be populated to allow this final result to be properly associated with the underlying data that generated it.

There are two ways to report sample reanalysis data:

1. If the laboratory reports two complete sets of final results, two SamplePlusMethod nodes should be used.

2. If the laboratory picks one 'best' result for each final reported analyte, then one SamplePlusMethod node would be used. The LabAnalysisID data element would be used to link each result to the correct underlying analysis. This is the preferred and most common approach used. If the data requester requires all potential results in addition to the laboratory selected 'best' result(s), then all results can be reported in Analyte nodes under each respective Analysis node.

Example 4-4, derived from the SW-846 Inorganics data, illustrates how final results can be reported for one water sample when an initial and diluted analysis has been performed on a single sample. In this example, the laboratory is using a single SamplePlusMethod node and is reporting the 'best' analyte value for each analyte reported in ReportedResult nodes. In addition, the laboratory is reporting the results from each analysis in Analyte nodes. Note that the final results for Magnesium are being reported from the original analysis (where the LabAnalysisID data element has the reported value 'Run-1') and the final results for Calcium are being reported from the diluted analysis (where the LabAnalysisID data element has the reported value 'Run-2'). Also note that the PreparationPlusCleanup node is identical under both Analysis nodes. Each Analysis node must contain all of the methods and processes that were performed on it.

Example 4-4.

```
<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <LabSampleID>070917-006</LabSampleID>
   <MatrixID>Water</MatrixID>
   <QCType>Field_Sample</QCType>

   <!-- Original undiluted analysis.-->

   <Analysis>
      <LabAnalysisID>Run-1</LabAnalysisID>
      <ClientMethodID>6010C</ClientMethodID>
      <AnalyzedDate>2007-12-10T14:45:00</AnalyzedDate>
      <DilutionFactor>1.0</DilutionFactor>
      <ResultBasis>Total</ResultBasis>

      <PreparationPlusCleanup>
         <PreparationPlusCleanupType>Preparation
         </PreparationPlusCleanupType>
         <ClientMethodID>3010C</ClientMethodID>
```

```
         <AliquotAmount>50</AliquotAmount>
         <AliquotAmountUnits>mL</AliquotAmountUnits>
         <FinalAmount>50</FinalAmount>
         <FinalAmountUnits>mL</FinalAmountUnits>
         <PreparedDate>2007-12-08</PreparedDate>
      </PreparationPlusCleanup>

      <!-- Original analysis.results are all reported here -->

      <Analyte>
         <ClientAnalyteID>7440-70-2</ClientAnalyteID>
         <ClientAnalyteName>Calcium</ClientAnalyteName>
         <Result>1430</Result>
         <ResultType>=</ResultType>
         <ResultUnits>mg/L</ResultUnits>
      </Analyte>
      <Analyte>
         <ClientAnalyteID>7439-95-4</ClientAnalyteID>
         <ClientAnalyteName>Magnesium</ClientAnalyteName>
         <Result>760</Result>
         <ResultType>=</ResultType>
         <ResultUnits>mg/L</ResultUnits>
      </Analyte>

   </Analysis>

   <!-- Diluted analysis -->

   <Analysis>
      <LabAnalysisID>Run-2</LabAnalysisID>
      <ClientMethodID>6010C</ClientMethodID>
      <AnalyzedDate>2007-12-10T15:45:00</AnalyzedDate>
      <DilutionFactor>2.0</DilutionFactor>
      <ResultBasis>Total</ResultBasis>

      <PreparationPlusCleanup>
         <PreparationPlusCleanupType>Preparation
         </PreparationPlusCleanupType>
         <ClientMethodID>3010C</ClientMethodID>
         <AliquotAmount>50</AliquotAmount>
         <AliquotAmountUnits>mL</AliquotAmountUnits>
         <FinalAmount>50</FinalAmount>
         <FinalAmountUnits>mL</FinalAmountUnits>
         <PreparedDate>2007-12-08</PreparedDate>
      </PreparationPlusCleanup>

      <!-- Diluted analysis.results are all reported here -->

      <Analyte>
         <ClientAnalyteID>7440-70-2</ClientAnalyteID>
         <ClientAnalyteName>Calcium</ClientAnalyteName>
         <Result>1420</Result>
         <ResultType>=</ResultType>
         <ResultUnits>mg/L</ResultUnits>
      </Analyte>
      <Analyte>
         <ClientAnalyteID>7439-95-4</ClientAnalyteID>
         <ClientAnalyteName>Magnesium</ClientAnalyteName>
         <Result>750</Result>
         <ResultType>=</ResultType>
```

```
          <ResultUnits>mg/L</ResultUnits>
       </Analyte>

    </Analysis>

    <!-- Final Results -->

    <ReportedResult>
       <ClientAnalyteID>7440-70-2</ClientAnalyteID>
       <ClientAnalyteName>Calcium</ClientAnalyteName>
       <LabAnalysisID>Run-2</LabAnalysisID>
       <Result>1420</Result>
       <ResultType>=</ResultType>
       <ResultUnits>mg/L</ResultUnits>
    </ReportedResult>
    <ReportedResult>
       <ClientAnalyteID>7439-95-4</ClientAnalyteID>
       <ClientAnalyteName>Magnesium</ClientAnalyteName>
       <LabAnalysisID>Run-1</LabAnalysisID>
       <Result>760</Result>
       <ResultType>=</ResultType>
       <ResultUnits>mg/L</ResultUnits>
    </ReportedResult>

 </SamplePlusMethod>
```

4.2 Relationships

The analytical relationships within the SEDD Specification are used to link each reported sample result back to the underlying processes that were used to generate or evaluate that result.

4.2.1 Batches

The SEDD Specification uses the concept of a batch as the primary mechanism for associating QC samples with regular ones. Analytical data review requires this association to assess the impact of QC sample performance to the quality of the regular sample results. For example, when doing volatiles by GC/MS, it is common practice to tune the instrument and verify the calibration once every shift. In this case, the SEDD Specification uses the concept of the Analysis batch to associate all the analyses done in one shift. The two Instrument QC analyses (tune and calibration verification) are associated with all regular and Method QC sample analyses in that shift by having a common value for the AnalysisBatch data element that occurs in each of their Analysis nodes.

The actual value used for the AnalysisBatch data element corresponding to one shift is not specified by the SEDD Specification, only that the value must be the same for all analyses in one shift and different for analyses in different shifts. The basis of the value for the AnalysisBatch data element must be given in the instructions provided by the data requester.

The SEDD Specification uses the following eleven (11) data elements to define Batches:

AnalysisBatch	A group of analyses done on one instrument under the control of one continuing calibration or continuing calibration verification. Calibration is used in a generic sense. The details of what defines an AnalysisBatch depends on the method. A given AnalysisBatch may contain one or more InstrumentQC samples and always refers to the InstrumentQC sample(s) that begin the analytical sequence.
AnalysisBatchEnd	Similar to the AnalysisBatch. A given AnalysisBatchEnd may contain one or more InstrumentQC samples and always refers to the InstrumentQC sample(s) that end the analytical sequence, if used by the method. The AnalysisBatch and AnalysisBatchEnd data elements for a given sample can never have the same value within a given analytical sequence for a given method.
PreparationBatch	A group of aliquots prepared together for analysis by one method. 'Together' can imply similarity of the time, place, and manner of preparation, with details depending on the method. The notion of preparation is used in a generic sense for any activity prior to instrumental analysis. Method blanks and/or Laboratory Control Samples are often used to demonstrate that the laboratory's process is in control in each PreparationBatch.
HandlingBatch	A group of samples, not aliquots, handled together during the initial processing for analysis by one method. A TCLP apparatus blank is often used to demonstrate that the handling process is in control.
CleanupBatch	A group of aliquots going through a cleanup step together as part of preparation for analysis by one method. This process could involve the use of Gel Permeation Chromatography (GPC) to cleanup a group of organic extracts.
RunBatch	A group of analyses done on one instrument under the control of one initial calibration. Calibration is used in a generic sense. The details of what defines RunBatch depend on the method. Typically, one RunBatch includes the analyses from one or more analysis batches.
MethodBatch	A group of samples, not aliquots, with similar matrices, analyzed by one method and expected to have similar response to the method. Matrix spikes and duplicates are typical types of QC associated with a MethodBatch.
LabReportingBatch	A group of samples reported as a unit (e.g., a CLP Sample Delivery Group). This batch is often used to define the context for definition (uniqueness) of batch values in data generated by the laboratory.
StorageBatch	A group of samples that are stored together. Volatile Organic Compound (VOC) refrigerator blanks are examples of QC associated with a StorageBatch.
ShippingBatch	A group of samples shipped in one container, such as a crate, cooler, or ice chest. Trip and temperature blanks are examples of QC associated with a ShippingBatch.

EquipmentBatch	A group of samples collected using the same equipment in a defined period of time. Rinsate blanks are examples of QC associated with an EquipmentBatch.
SamplingBatch	A group of samples collected together. Field blanks are examples of QC associated with a SamplingBatch.

Example 4-5 shows how a regular field sample is linked to the preparation, run, and analysis batches as part of a typical daily run sequence when implemented according to SW-846 Method 8270 (Semivolatile) rules. The sequence starts with a Tune and Continuing Calibration Verification InstrumentQC samples. It is then followed by a Method Blank and a sample.

Example 4-5.

```
<!-- First daily tune: -->

<InstrumentQC>
   <ClientMethodID>8270C</ClientMethodID>
   <QCType>Instrument_Performance_Check_Tune</QCType>
   <LabInstrumentQCID>Tune-2</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
   </Analysis>

</InstrumentQC>

<!-- First daily continuing calibration verification: -->

<InstrumentQC>
   <ClientMethodID>8270C</ClientMethodID>
   <QCType>Continuing_Calibration_Verification</QCType>
   <LabInstrumentQCID>CCV-1</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
   </Analysis>

</InstrumentQC>

<!-- Method blank: -->

<SamplePlusMethod>
   <ClientMethodID>8270C</ClientMethodID>
   <QCType>Method_Blank</QCType>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>

      <PreparationPlusCleanup>
         <PreparationBatch>First Preparation Batch</PreparationBatch>
      </PreparationPlusCleanup>

   </Analysis>
```

```
</SamplePlusMethod>

<!-- Regular sample: -->

<SamplePlusMethod>
   <ClientMethodID>8270C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <QCType>Field_Sample</QCType>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>

      <PreparationPlusCleanup>
         <PreparationBatch>First Preparation Batch</PreparationBatch>
      </PreparationPlusCleanup>

   </Analysis>
</SamplePlusMethod>
```

As shown in Example 4-5, the Client Sample ID “Sample-01” is linked to three batches as follows:

- To the initial calibration by the data element RunBatch containing the value ‘First Run Batch.’
- To the continuing calibration verification and associated tune by the data element AnalysisBatch containing the value ‘First Analysis Batch.’
- To the Method QC sample (Method Blank) by the data element PreparationBatch containing the value ‘First Preparation Batch.’

Example 4-6 shows how regular field samples are linked to the preparation, run, and analysis batches as part of a typical daily run sequence when implemented according to SW-846 Method 6010 (ICP/AES) Metals’ rules. The sequence starts with Continuing Calibration Verification and Continuing Calibration Verification Blank InstrumentQC samples. It is then followed by a Method Blank and a sample. A second analysis sequence is then performed followed by the analysis of a second sample. The sequence is then terminated with closing Continuing Calibration Verification and Continuing Calibration Verification Blank InstrumentQC samples.

Example 4-6.

```
<!-- Opening Continuing Calibration Verification InstrumentQC
standard: -->

<InstrumentQC>
   <ClientMethodID>6010C</ClientMethodID>
   <QCType>Continuing_Calibration_Verification</QCType>
   <LabInstrumentQCID>CCV-1</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>First Analysis Batch</AnalysisBatchEnd>
```

```
   </Analysis>

</InstrumentQC>

<!-- Opening Continuing Calibration Blank InstrumentQC standard: -->

<InstrumentQC>
   <ClientMethodID>6010C</ClientMethodID>
   <QCType>Continuing_Calibration_Blank</QCType>
   <LabInstrumentQCID>CCB-1</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>First Analysis Batch</AnalysisBatchEnd>
   </Analysis>

</InstrumentQC>

<!-- Method blank: -->

<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <QCType>Method_Blank</QCType>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Second Analysis Batch</AnalysisBatchEnd>

      <PreparationPlusCleanup>
         <PreparationBatch>First Preparation Batch</PreparationBatch>
      </PreparationPlusCleanup>
   </Analysis>
</SamplePlusMethod>

<!-- First Regular sample: -->

<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <QCType>Field_Sample</QCType>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>First Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Second Analysis Batch</AnalysisBatchEnd>

      <PreparationPlusCleanup>
      <PreparationBatch>First Preparation Batch</PreparationBatch>
      </PreparationPlusCleanup>

   </Analysis>
</SamplePlusMethod>

<!-- Middle Continuing Calibration Verification InstrumentQC
standard: -->
```

```
<InstrumentQC>
   <ClientMethodID>6010C</ClientMethodID>
   <QCType>Continuing_Calibration_Verification</QCType>
   <LabInstrumentQCID>CCV-2</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>Second Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Second Analysis Batch</AnalysisBatchEnd>
   </Analysis>
</InstrumentQC>

<!-- Middle Continuing Calibration Blank InstrumentQC standard: -->

<InstrumentQC>
   <ClientMethodID>60100C</ClientMethodID>
   <QCType>Continuing_Calibration_Blank</QCType>
   <LabInstrumentQCID>CCB-2</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>Second Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Second Analysis Batch</AnalysisBatchEnd>
   </Analysis>
</InstrumentQC>

<!-- Second Regular sample: -->

<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <ClientSampleID>Sample-02</ClientSampleID>
   <QCType>Field_Sample</QCType>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>Second Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Third Analysis Batch</AnalysisBatchEnd>

      <PreparationPlusCleanup>
         <PreparationBatch>First Preparation Batch</PreparationBatch>
      </PreparationPlusCleanup>

   </Analysis>
</SamplePlusMethod>

<!-- Closing Continuing Calibration Verification InstrumentQC
standard: -->

<InstrumentQC>
   <ClientMethodID>6010C</ClientMethodID>
   <QCType>Continuing_Calibration_Verification</QCType>
   <LabInstrumentQCID>CCV-3</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>Third Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Third Analysis Batch</AnalysisBatchEnd>
   </Analysis>
```

```
</InstrumentQC>

<!-- Closing Continuing Calibration Blank InstrumentQC standard: -->

<InstrumentQC>
   <ClientMethodID>60100C</ClientMethodID>
   <QCType>Continuing_Calibration_Blank</QCType>
   <LabInstrumentQCID>CCB-3</LabInstrumentQCID>

   <Analysis>
      <RunBatch>First Run Batch</RunBatch>
      <AnalysisBatch>Third Analysis Batch</AnalysisBatch>
      <AnalysisBatchEnd>Third Analysis Batch</AnalysisBatchEnd>
   </Analysis>
</InstrumentQC>
```

As shown in Example 4-6, the Client Sample ID ‘Sample-01’ is linked to three batches as follows:

- To the initial calibration by the data element RunBatch containing the value ‘First Run Batch.’

- To the opening continuing calibration verification standard and associated blank by the data element AnalysisBatch containing the value ‘First Analysis Batch.’ To the closing continuing calibration verification standard and associated blank by the data element AnalysisBatchEnd containing the value ‘Second Analysis Batch.’

- To the Method QC sample (Method Blank) by the data element PreparationBatch containing the value ‘First Preparation Batch.’

4.2.2 Analysis Groups

Some methods may require several analyses to calculate one result (e.g., Total Organic Carbon (TOC), method of standard additions). Further, some methods may allow several potential results to be calculated, with an average final result selected for reporting as the ‘final result.’

The SEDD Specification uses AnalysisGroup nodes under the SamplePlusMethod node to associate several analyses underlying one set of possible results.

AnalysisGroup nodes under the InstrumentQC node are also used to link several analyses (e.g., multipoint initial calibrations) that are part of one instrument QC process.

The AnalysisGroupID data element must be present in the following three nodes - AnalysisGroup, Analysis, and ReportedResult.

Example 4-7 is an example of an XML file that reports initial calibration data which has multiple analyses. This example, derived from the analysis of semivolatile organics using SW-846 Method 8270, illustrates how analyses in one initial calibration might be reported using ONLY the Analysis and AnalysisGroup nodes (does not go below into the Analyte nodes).

Example 4-7.

```
<InstrumentQC>
   <ClientMethodID>8270C</ClientMethodID>
   <LabInstrumentQCID>ICAL-1</LabInstrumentQCID>
   <QCType>Initial_Calibration</QCType>

   <!-- 1st standard used for initial calibration. -->

   <Analysis>
      <LabAnalysisID>SV202</LabAnalysisID>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>RRF-010</AnalysisType>
      <AnalyzedDate>2007-11-20T12:50</AnalyzedDate>
      <InstrumentID>GCMS1</InstrumentID>
      <!--Individual RRFs would go in Analyte nodes nested here:-->
   </Analysis>

   <!-- 2nd standard used for initial calibration. - ->

   <Analysis>
      <LabAnalysisID>SV203</LabAnalysisID>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>RRF-020</AnalysisType>
      <AnalyzedDate>2007-11-20T13:50</AnalyzedDate>
      <InstrumentID>GCMS1</InstrumentID>
      <!--Individual RRFs would go in Analyte nodes nested here:-->
   </Analysis>

   <!-- 3rd standard used for initial calibration. -->

   <Analysis>
      <LabAnalysisID>SV204</LabAnalysisID>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>RRF-050</AnalysisType>
      <AnalyzedDate>2007-11-20T14:50</AnalyzedDate>
      <InstrumentID>GCMS1</InstrumentID>
      <!--Individual RRFs would go in Analyte nodes nested here:-->
   </Analysis>

   <!-- 4th standard used for initial calibration. -->

   <Analysis>
      <LabAnalysisID>SV205</LabAnalysisID>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>RRF-080</AnalysisType>
      <AnalyzedDate>2007-11-20T15:50</AnalyzedDate>
      <InstrumentID>GCMS1</InstrumentID>
      <!--Individual RRFs would go in Analyte nodes nested here:-->
   </Analysis>

   <!-- 5th standard used for initial calibration. -->

   <Analysis>
      <LabAnalysisID>SV206</LabAnalysisID>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>RRF-160</AnalysisType>
      <AnalyzedDate>2007-11-20T16:50</AnalyzedDate>
      <InstrumentID>GCMS1</InstrumentID>
      <!--Individual RRFs would go in Analyte nodes nested here:-->
```

```
   </Analysis>

      <!-- The AnalysisGroup node reports the calibration curve
      characteristics-->

   <AnalysisGroup>
      <AnalysisGroupID>ICAL01</AnalysisGroupID>
      <AnalysisType>Initial_Calibration</AnalysisType>
      <!-- Mean RRFs and RSDs would go in Analyte nodes nested here:
      -->
   </AnalysisGroup>

</InstrumentQC>
```

Example 4-8, derived from the SW-846 Inorganics data, illustrates a complex method requiring an AnalysisGroup node. Data is shown for one analyte and many less important data elements are omitted. In this example, the method of standard additions (MSA) was performed on the field soil sample. Intermediate results are actually reported in the Analyte nodes rather than final Results for each analysis. Intermediate results are results obtained directly from the initial calibration curve (in liquid units) with no corrections made for the aliquot amount taken or Percent Moisture in the original sample.

Example 4-8.

```
<!-- Regular soil sample - GFAA Method with MSA data included: -->

<SamplePlusMethod>
   <ClientMethodID>7841</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <LabSampleID>070917-011</LabSampleID>
   <MatrixID>Soil</MatrixID>
   <QCType>Field_Sample</QCType>

   <!-- Final result: -->

   <ReportedResult>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <ClientAnalyteID>7440-28-0</ClientAnalyteID>
      <ClientAnalyteName>Thallium</ClientAnalyteName>
      <Result>1.58</Result>
      <ResultType>=</ResultType>
      <ResultUnits>mg/kg</ResultUnits>
   </ReportedResult>

   <!-- ANALYSIS GROUP for MSA -->

   <AnalysisGroup>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <AnalysisType>MSA</AnalysisType>
   </AnalysisGroup>

   <!-- First MSA analysis -->

   <Analysis>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <LabAnalysisID>GFAA-TL1-071015-28</LabAnalysisID>
      <AnalysisType>MSA-0</AnalysisType>
```

```
      <Analyte>
         <ClientAnalyteID>7440-28-0</ClientAnalyteID>
         <IntermediateResult>7.6</IntermediateResult>
         <IntermediateResultUnits>ug/L</IntermediateResultUnits>
      </Analyte>
   </Analysis>

   <!-- Second MSA analysis: -->

   <Analysis>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <LabAnalysisID>GFAA-TL1-071015-29</LabAnalysisID>
      <AnalysisType>MSA-1</AnalysisType>

      <Analyte>
         <ClientAnalyteID>7440-28-0</ClientAnalyteID>
         <IntermediateResult>13</IntermediateResult>
         <IntermediateResultUnits>ug/L</IntermediateResultUnits>
      </Analyte>
   </Analysis>
   <!-- Third MSA analysis: -->

   <Analysis>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <LabAnalysisID>GFAA-TL1-071015-30</LabAnalysisID>
      <AnalysisType>MSA-2</AnalysisType>

      <Analyte>
         <ClientAnalyteID>7440-28-0</ClientAnalyteID>
         <IntermediateResult>17</IntermediateResult>
         <IntermediateResultUnits>ug/L</IntermediateResultUnits>
      </Analyte>
   </Analysis>

   <!-- Fourth MSA analysis: -->

   <Analysis>
      <AnalysisGroupID>First Analysis Group</AnalysisGroupID>
      <LabAnalysisID>GFAA-TL1-071015-31</LabAnalysisID>
      <AnalysisType>MSA-3</AnalysisType>

      <Analyte>
         <ClientAnalyteID>7440-28-0</ClientAnalyteID>
         <IntermediateResult>21</IntermediateResult>
         <IntermediateResultUnits>ug/L</IntermediateResultUnits>
      </Analyte>
   </Analysis>
</SamplePlusMethod>
```

As shown in Example 4-8, the Client Sample ID ‘Sample-01’ has been analyzed using the Method of Standard Additions (MSA). The final Thallium Result was reported as ‘1.58’ with ResultUnits ‘mg/kg.’ The final reported result is linked to the data element AnalysisGroupID with a value of ‘First Analysis Group’ instead of to a single analysis (which would have used the data element LabAnalysisID). All the MSA Analyses are similarly linked to each other and the final result through the same AnalysisGroupID data element having the value ‘First Analysis Group.’

4.2.3 Analyte Groups

Some methods may require the reporting of an analyte that is not directly measured by a given method where the reported analyte is actually the combination of two or more analytes that are directly measured by the method (e.g., Hardness, where the reported analyte Hardness is actually the summed values of the Calcium and Magnesium measured analytes).

The SEDD Specification uses AnalyteGroup nodes under the Analysis node to associate two or more analytes that are directly measured using the method(s) indicated to report an analyte that typically cannot be measured directly.

The AnalyteGroupID data element must be present in the following three nodes - AnalyteGroup, Analyte, and ReportedResult.

Example 4-9, derived from SW-846 Inorganics data, illustrates a method requiring the AnalyteGroup node. Data is shown for only two measured analytes and many less important data elements are omitted. In this example, a single analysis was performed on the field water sample ‘Sample-01’ and a final result was reported for ‘Hardness.’

Example 4-9.

```
<!-- Regular water sample - ICP Method: -->

<SamplePlusMethod>
   <ClientMethodID>6010B</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <LabSampleID>040817-010</LabSampleID>
   <MatrixID>Water</MatrixID>
   <QCType>Field_Sample</QCType>

   <!-- Final result: -->

   <ReportedResult>
      <AnalyteGroupID>First Analyte Group</AnalyteGroupID>
      <ClientAnalyteID>E1643592</ClientAnalyteID>
      <ClientAnalyteName>Hardness</ClientAnalyteName>
      <Result>28</Result>
      <ResultType>=</ResultType>
      <ResultUnits>mg/L</ResultUnits>
   </ReportedResult>

   <Analysis>
      <LabAnalysisID>ICP-071015-28</LabAnalysisID>
      <AnalysisType>Initial</AnalysisType>

      <!-- ANALYTE GROUP for Hardness -->
      <AnalyteGroup>
         <AnalyteGroupID>First Analyte Group</AnalyteGroupID>
         <ClientAnalyteID>E1643592</ClientAnalyteID>
         <ClientAnalyteName>Hardness</ClientAnalyteName>
      </AnalyteGroup>

      <!-- First Analyte to be associated with Hardness -->

      <Analyte>
```

```
         <AnalyteGroupID>First Analyte Group</AnalyteGroupID>
         <ClientAnalyteName>Calcium</ClientAnalyteName>
         <ClientAnalyteID>7440-70-2</ClientAnalyteID>
         <Result>15</Result>
         <ResultType>=</ResultType>
         <ResultUnits>mg/L</ResultUnits>
      </Analyte>

      <!-- Second Analyte to be associated with Hardness -->

      <Analyte>
         <AnalyteGroupID>First Analyte Group</AnalyteGroupID>
         <ClientAnalyteName>Magnesium</ClientAnalyteName>
         <ClientAnalyteID>7439-95-4</ClientAnalyteID>
         <Result>13</Result>
         <ResultType>=</ResultType>
         <ResultUnits>mg/L</ResultUnits>
      </Analyte>
   </Analysis>
</SamplePlusMethod>
```

As shown in Example 4-9, the sample identified with ClientSampleID ‘Sample-01’ has been analyzed to determine its Hardness. The final Hardness Result was reported as ‘28’ with ResultUnits ‘mg/L.’ The final reported result is linked to a group of analytes rather than to a single measured analyte by using the data element AnalyteGroupID with a value of ‘First Analyte Group.’ All the Analytes that are associated with the final reported Hardness result are similarly linked to each other and the final result through this same data element AnalyteGroupID having the value ‘First Analyte Group.’

4.2.4 QC Categories and QC Linkage

The QCCategory and QCLinkage data elements (under the SamplePlusMethod and InstrumentQC nodes) support cross-program movement of data (e.g., supply data for processing by different site’s data validation programs) and development of implementation-independent EDD processing software. Because valid values for both the QCCategory and QCLinkage data elements are given in the SEDD Specification, processing software can ‘understand’ how to store, report, and associate a method-level QC sample.

The QCCategory data element specifies the type of QC values and comparisons appropriate to a method-level QC sample (one reportable in a SamplePlusMethod node). Valid values for the QCCategory data element include the following:

Blank	A QC sample made to contain negligible (or unmeasurable) quantities of the analyte(s) of interest. Detection of an analyte in a blank is an indication of contamination. Data is similar to that for a regular sample. This same QCCategory would be used with many QCTypes (e.g., those corresponding to method, trip, rinsate, field, and other types of implementation-defined blanks).
Blank_Spike	A QC sample with known amounts of target analytes added to a Blank. Data potentially includes a

	PercentRecovery and an ExpectedResult for each analyte for which the AnalyteType is Spike. An Interference Check Sample is a type of BlankSpike where the results for unspiked analytes are of interest.
Spike	A reanalysis of a regular sample done for QC purposes with known amounts of target analytes added to the sample. Data is expected to include an OriginalClientSampleID for each SamplePlusMethod node and, potentially, a PercentRecovery and an ExpectedResult for each analyte for which the AnalyteType is Spike. The OriginalClientSampleID identifies the original sample that was spiked.
Duplicate	A reanalysis of a regular sample done for QC purposes. Data is expected to include an OriginalClientSampleID for each SamplePlusMethod node and, potentially, an RPD for each analyte. The OriginalClientSampleID identifies the original sample that was reanalyzed. This use of Duplicate is meant to include what are called ‘splits’ or ‘replicates’, as long as only two sets of results are involved.
Serial_Dilution	A diluted reanalysis of a regular sample done for QC purposes. Data is expected to include an OriginalClientSampleID and, potentially, a PercentDifference. The OriginalClientSampleID identifies the original sample that was diluted then reanalyzed.
Blank_Spike_Duplicate	A second analysis of a BlankSpike. Data is expected to include an OriginalLabSampleID, and, potentially, a PercentRecovery, an RPD and an ExpectedResult for each analyte for which the AnalyteType is ‘Spike.’ The OriginalLabSampleID identifies the original Blank_Spike that was reanalyzed.
Spike_Duplicate	A second reanalysis of a regular sample done for QC purposes with a known spike added. Data is expected to include an OriginalClientSampleID, and, potentially, a PercentRecovery, an RPD and an ExpectedResult for each analyte where the AnalyteType is ‘Spike.’ The OriginalClientSampleID identifies the regular sample that was spiked and reanalyzed. There should be another SamplePlusMethod node with QCCategory ‘Spike’ with the same ClientMethodID and OriginalClientSampleID.
Non-Client_Sample	This type of QC sample is different than the other QC sample types normally encountered in that it is, simply, a regular sample. Many programs require that certain data be reported from the analysis of non-client samples that were prepared or analyzed with project-specific samples. This is often done to verify run sequences and to ensure that certain QC samples were analyzed at an appropriate frequency. The actual analytical results rarely would be reported.

The QCLinkage data element specifies the type of batch used to make associations for a QC sample and the following applies:

- Allowed valid values for the QCLinkage data element are the names of the various batch fields defined by the SEDD Specification. They are AnalysisBatch, PreparationBatch, HandlingBatch, CleanupBatch, RunBatch, MethodBatch, LabReportingBatch, StorageBatch, ShippingBatch, EquipmentBatch and SamplingBatch (as given in Section 4.2.1). Because there are potentially multiple handling nodes for each sample, if the QCLinkage data element value is HandlingBatch, a ClientMethodID or HandlingType data element must be specified for the QC sample to make the linkage unambiguous. Similarly, a ClientMethodID or CleanupType data element must be specified if the QCLinkage data element value is CleanupBatch.

- The limited list of valid values for QCCategory and QCLinkage data elements are part of the SEDD Specification. They represent a choice about the types of data expected to be reported. This choice enables the development of reasonably method-independent database software to support performance-based verification and validation of analytical data.

As an example, in a SamplePlusMethod node, if the QCType data element value is Lab_Duplicate, the QCCategory data element value is Duplicate, and the QCLinkage data element value is MethodBatch, then a reader will know this data is for a client-defined type of QC called a Lab_Duplicate. The reader will also know it is processed with rules typical for Duplicates and it is to be associated with other SamplePlusMethod nodes with the same value for the MethodBatch data element.

Example 4-10 shows how the QCCategory and QCLinkage data elements in the EDD help to show the type of sample being analyzed (e.g., Blank) and the linkage to a batch (e.g., Preparation) in an Inorganics analysis:

Example 4-10.

```
<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <LabSampleID>ICP-WG2413-1</LabSampleID>
   <MatrixID>Soil</MatrixID>
   <QCCategory>Blank</QCCategory>
   <QCLinkage>PreparationBatch</QCLinkage>
   <QCType>Method_Blank</QCType>

   <Analysis>
      <PreparationPlusCleanup>
         <PreparationBatch>ICP-WG2413-A</PreparationBatch>
      </PreparationPlusCleanup>
   </Analysis>
</SamplePlusMethod>
```

A general EDD reader might not recognize the ClientMethodID data element value (6010C, specified by a specific implementation) and hence not know the meaning of the QCType data element value (Method_Blank) or even that this is ICP inorganics data. However, based on the QCCategory data element value (Blank) it knows to use ‘blank-like’ rules to process this data. Based on the QCLinkage data element value

(PreparationBatch) it knows to associate this QC sample with other analyses with the same value (ICP-WG2413-A) for the PreparationBatch data element.

4.2.5 Comparisons

There are two basic types of comparisons that are allowed in the SEDD Specification - Analyte Comparisons and Peak Comparisons.

Analyte Comparison

- Analyte comparisons are used to describe the effects of potentially interfering analytes on the measured analyte peak.
- Data from instrument QC checks for cross-analyte interference are reported in the AnalyteComparison node.
- A common use of AnalyteComparison node is in the reporting of ICP Interelement Correction factors where the contribution to the analyte measurement from interfering analytes is reported in data elements in AnalyteComparison nodes under a Peak node (see Appendix B, Figure 4).

Example 4-11 illustrates how a data generator would report the Inter Element Correction factors (IECs) for a typical ICP/AES method.

Example 4-11.

```
<!-- ICP Interelement Correction Factors: -->

<SamplePlusMethod>
   <ClientMethodID>6010C</ClientMethodID>
   <ClientSampleID>Sample-01</ClientSampleID>
   <MatrixID>Water</MatrixID>
   <QCType>Field_Sample</QCType>

   <Analysis>
      <LabAnalysisID>P2_ICP_042694</LabAnalysisID>

      <!-- Report interference with this analyte: -->

      <Analyte>
         <ClientAnalyteID>7439-92-1</ClientAnalyteID>
         <ClientAnalyteName>Lead</ClientAnalyteName>

         <!-- At this peak: -->

         <Peak>
            <PeakID>220</PeakID>
            <Wavelength>220.35</Wavelength>
            <WavelengthUnits>nm</WavelengthUnits>

            <!-- First interferent: -->
            <AnalyteComparison>
   <ClientAnalyteID>7429-90-5</ClientAnalyteID>
               <ClientAnalyteName>Aluminum</ClientAnalyteName>
               <CorrectionFactor>0.000370</CorrectionFactor>
```

```
            </AnalyteComparison>
         </Peak>
      </Analyte>
   </Analysis>
</SamplePlusMethod>
```

As shown in Example 4-11, during the analysis of Lead by ICP-AES, Aluminum is an interferent. Lead is identified as an analyte under the Analyte node using the data element ClientAnalyteName. The Peak used for measurement of Lead is identified in the Peak node by the data element PeakID. Aluminum interferes with this peak and its interelement correction factor is reported in the AnalyteComparison node using the data element CorrectionFactor.

Peak Comparison

- Peak comparisons are used to compare measurements made at two or more different peaks. Peak comparisons can describe cross-peak comparisons within the same analyte (e.g., abundance ratios for tunes), between two analytes (e.g., calculating the relative response factor (RRF) for initial and continuing calibrations or inter-peak resolutions in chromatography).

- Data from these peak comparisons are reported in the PeakComparison node (see Appendix B, Figure 4).

One common example for using PeakComparison nodes is for the reporting of GC/MS tune data where only a single analyte is involved.

Example 4-12.

```
<!-- Part of the data for one tune: -->

<InstrumentQC>
   <ClientMethodID>8270C</ClientMethodID>
   <QCType>Instrument_Performance_Check_Tune</QCType>
   <LabInstrumentQCID>Tune 1</LabInstrumentQCID>

   <Analysis>
      <LabAnalysisID>SV417</LabAnalysisID>

      <Analyte>
      <ClientAnalyteID>5074-71-5</ClientAnalyteID>
      <ClientAnalyteName>DFTPP</ClientAnalyteName>
      <AnalyteType>System_Monitoring_Compound</AnalyteType>

         <!-- One mass spectral peak: -->

         <Peak>
         <PeakID>68</PeakID>

            <!-- First comparison: -->

            <PeakComparison>
               <PeakID>198</PeakID>
               <PercentRatio>0.0</PercentRatio>
            </PeakComparison>
```

```
            <!-- Second Comparison: -->

            <PeakComparison>
               <PeakID>69</PeakID>
               <PercentRatio>0.0</PercentRatio>
            </PeakComparison>
         </Peak>
      </Analyte>
   </Analysis>
</InstrumentQC>
```

As shown in Example 4-12, a DFTPP tune (for method SW-846 8270 semivolatile organics) is being reported under the Analyte node using the data element AnalyteName. The peak (mass number 68) to be evaluated is identified under the Peak node using the data element PeakID. This peak (mass number 68) is compared to the following two peaks (mass numbers 198 and 69) under separate PeakComparison nodes using the data element PeakID. The data element PercentRatio is used to report the actual comparison (expressed as a percent ratio).

This page intentionally left blank.

APPENDIX A
DATA ELEMENT DICTIONARY (DED)

NOTE: For those data elements that have the format 'Limited List', the list of valid values is provided in a separate document.

DATA ELEMENT	DESCRIPTION

AliquotAmount

Format: Numeric

Type:

Definition: The amount (weight or volume) of sample subjected to an analysis. The final results for any given analysis are based on the AliquotAmount used.

Applicable Node(s):

Analysis The amount of sample used for this analysis.

PreparationPlusCleanup If the analytical method requires the prior use of an independent preparative method, then the AliquotAmount is the amount of sample subjected to the preparative method prior to actual analysis of the sample.

AliquotAmountUnits

Format: Limited List

Type:

Definition: Units for AliquotAmount

Applicable Node(s):

Analysis

PreparationPlusCleanup

AlternateLabAnalysisID

Format: Identifier

Type:

Definition: An alternate laboratory identifier for an analysis.

Applicable Node(s):

Analysis This value is for information purposes only to facilitate tracking back into the laboratory's systems.

DATA ELEMENT	DESCRIPTION
AlternateLabSampleID	
Format: Identifier	
Type:	
Definition:	An alternate laboratory identifier for a sample.
Applicable Node(s):	
SamplePlusMethod	This value is for information purposes only to facilitate tracking back into the laboratory's systems. It might be used when the laboratory has both a laboratory-wide sample ID and a different, department specific one for particular methods.
AmountAdded	
Format: Numeric	
Type:	
Definition:	The amount (weight or volume) of an analyte that has been spiked into a sample aliquot or standard, or used to prepare a standard, at any time during the analytical process.
Applicable Node(s):	
Analyte	Specifies a known weight or volume of analyte that has been spiked into the sample aliquot or standard. The StandardConcentration data element must also be used to fully define the amount of analyte added. AmountAdded can refer to spikes, surrogates, tracers, internal standards, etc. where known amounts of an analyte or analytes have been added to samples and standards for QC purposes. When a standard is being prepared, this specifies a known weight or volume of analyte that is used to prepare the standard. The StandardConcentration and StandardFinalVolume data elements must also be used to fully define the final concentration of the analyte in the prepared standard. This is often used to describe the preparation of initial calibration, continuing calibration verification or other InstrumentQC standards where more standard is prepared than will actually be consumed during a single analysis.

DATA ELEMENT	DESCRIPTION

AmountAddedLocation

Format: Limited List

Type:

Definition: The specific step in the process where an analyte is added.

Applicable Node(s):

Analyte Analyte(s) may be spiked directly into an original sample aliquot or into a digested/extracted aliquot or at other times during the processing of a sample aliquot or a standard or during the preparation of a standard.

AmountAddedUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the AmountAdded, by which the AmountAdded may differ from the true value due to this specific process.

Applicable Node(s):

Analyte Expressed as an offset to the AmountAdded (y) in the form: AmountAdded ± positive numeric value ($y \pm a$).

AmountAddedUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, at which the AmountAddedUncertainty was determined.

Applicable Node(s):

Analyte Reported as a value between 0 and 100%.

DATA ELEMENT	DESCRIPTION

AmountAddedUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported AmountAddedUncertainty.

Applicable Node(s):

Analyte This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality); statistical experimental design (e.g., number of replicate measurements).

AmountAddedUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the AmountAdded.

Applicable Node(s):

Analyte Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the AmountAdded, ‘Other_Interval’ when the interval is not centered on the AmountAdded.

AmountAddedUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the AmountAdded may differ from the true value due to this specific process.

Applicable Node(s):

Analyte Expressed as a upper limit to the AmountAdded in the form: AmountAdded (y) < Upper AmountAdded limit (a_H). When both Upper and Lower AmountAdded limits are reported, the AmountAdded should appear as: Lower Limit AmountAdded (a_L) < AmountAdded (y) < Upper Limit AmountAdded (a_H).

DATA ELEMENT	DESCRIPTION

AmountAddedUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the AmountAdded may differ from the true value due to this specific process.

Applicable Node(s):

Analyte Expressed as a lower limit to the AmountAdded in the form: Lower AmountAdded limit (a_L) < AmountAdded (y). When both Upper and Lower AmountAdded limits are reported, the AmountAdded should appear as: Lower Limit AmountAdded (a_L) < AmountAdded (y) < Upper Limit AmountAdded (a_H).

AmountAddedUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the AmountAddedUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

Analyte Example Valid Values: ‘Category A’ where the estimate of the AmountAddedUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the AmountAddedUncertainty is determined using some other method (in whole or in part).

AmountAddedUncertaintyUnits

Format: Limited List

Type:

Definition: Units for AmountAddedUncertainty.

Applicable Node(s):

Analyte If the client specifies that the AmountAddedUncertaintyUnits must be the same as the AmountAddedUnits, the AmountAddedUncertaintyUnits need not be specified.

DATA ELEMENT	DESCRIPTION

AmountAddedUnits

Format: Limited List

Type:

Definition: Units for AmountAdded.

Applicable Node(s):

Analyte

Analysis

Format:

Type:

Definition: A parent data element that describes one complete sequence of events, from taking a sample aliquot through the measurement process, as defined as part of one method.

Applicable Node(s)

InstrumentQC

SamplePlusMethod

DATA ELEMENT	DESCRIPTION
AnalysisBatch	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier that is used to link multiple analyses done on one instrument, associated with one or more instrument quality control samples, at which the instrument is checked to be in control at the beginning of an analysis sequence.
Applicable Node(s):	
Analysis	Example: Analyses QC'd by the same continuing calibration verification or similar InstrumentQC that is run at the beginning of an analysis sequence. One or more InstrumentQC sample(s) may be used to start a given analysis batch and all of the regular sample(s) and associated InstrumentQC sample(s) would be represented by the same laboratory assigned identifier. If one or more InstrumentQC sample(s) only open a given analytical sequence, then the AnalysisBatchEnd data element may not be required. If one or more InstrumentQC samples only open a new analytical sequence or both open a new analytical sequence and close out a prior analytical sequence, then both the AnalysisBatch and AnalysisBatchEnd data elements would be used and both would be populated with the same value. For regular or MethodQC samples, the AnalysisBatch data element would be populated with the value of the AnalysisBatch data element of the InstrumentQC sample(s) that opened the analytical sequence.

DATA ELEMENT	DESCRIPTION

AnalysisBatchEnd

Format: Identifier

Type:

Definition: A laboratory-defined identifier that is used to link multiple analyses done on one instrument, associated with one or more instrument quality control samples, at which the instrument is checked to be in control at the end of the analysis sequence.

Applicable Node(s):

Analysis Example: Analyses QC'd by the same continuing calibration verification or similar InstrumentQC that is run at the end of an analysis sequence. One or more InstrumentQC sample(s) may be used to end any given analysis batch and all of the regular sample(s) and InstrumentQC sample(s) would be represented by the same laboratory assigned identifier. If one or more InstrumentQC sample(s) only close a given analytical sequence or both close out a prior analytical sequence and open a new analytical sequence, then both the AnalysisBatch and AnalysisBatchEnd data elements would be used and both would be populated with the same value. For regular or MethodQC samples, the AnalysisBatchEnd data element would be populated with the value of the AnalysisBatchEnd data element of the InstrumentQC sample(s) that closed the analytical sequence. If a given analytical sequence was not closed out by any InstrumentQC sample(s), then this data element would not be required.

AnalysisDuration

Format: Numeric

Type:

Definition: The length of time of the instrumental analysis.

Applicable Node(s):

Analysis Example: Radiochemical count time, ICP integration time.

Analyte The duration of the instrumental analysis for this analyte.

Peak The duration of the instrumental analysis for this peak.

PeakReplicate The duration of the instrumental analysis for this peak replicate.

DATA ELEMENT	DESCRIPTION

AnalysisDurationUnits

Format: Limited List

Type:

Definition: Units for AnalysisDuration.

Applicable Node(s):

Analysis

Analyte

Peak

PeakReplicate

AnalysisGroup

Format:

Type:

Definition: A parent data element that links calculated data associated with multiple analyses for one method.

Applicable Node(s):

InstrumentQC

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

AnalysisGroupID

Format: Identifier

Type: Required Conditionally

Definition:	A laboratory-defined identifier that is used to link multiple analyses performed on a single instrument to generate a single analyte result that is dependent upon each individual analysis.
Applicable Node(s):	
AnalysisGroup	Example: Analysis groups are used during initial calibration to determine average relative response or calibration factors or other calibration curve characteristics. They would normally be used to report this data for multi-point calibration curves. Analysis groups are used when the Method of Standard Additions is used to determine the concentration of a given analyte in a sample. Analysis groups are used when an average result is to be reported from multiple analyses.
Analysis	The AnalysisGroup this analysis is part of.
ReportedResult	The AnalysisGroup this final result was derived from.

AnalysisRequestID

Format: Identifier

Type:

Definition:	A client-defined identifier for the paperwork that authorizes the analyses of specific samples by listed methods.
Applicable Node(s):	
SamplePlusMethod	Can refer to a ‘Request for Analysis’ form that is usually different from the Chain-of-Custody form. Sometimes this is identical to the chain of custody identifier.

DATA ELEMENT	DESCRIPTION

AnalysisType

Format: Limited List

Type: Required

Definition: A term used to define the type of analysis (e.g., initial, confirmation, MSA). This term is also used to uniquely identify a single analysis from multiple analyses that are used to generate a single result.

Applicable Node(s):

Analysis Example Valid Values:

1. For a regular single analysis, the default Valid Value would be 'Initial.' For a regular single confirmation analysis, the default Valid Value would be 'Confirmation.'
2. During multipoint initial calibrations, this data element would be used to identify the individual analyses performed. Example Valid Value: 'RRF-#', 'CF-#', 'Standard-#' where '#' can be any number. The numerical part of each term could correspond to the concentration of the analyte in the standard or just simply the standard number.
3. If multiple analyses are averaged to produce a single final result, this data element would be used to identify the individual analyses performed. Example Valid Value: 'Replicate-#', where '#' can be any integer.
4. During use of the Method of Standard Additions, this data element would be used to identify the individual analyses performed. Example Valid Value: 'MSA-#,' where '#' can be any integer.
5. When dilutions, reinjections or reanalyses are performed, this data element would be used to identify the individual analyses performed. Example Valid Values: 'Reanalysis-#', 'Reinjection-#', 'Dilution-#', where '#' can be any integer. A 'Reinjection' involves taking a previously processed aliquot and repeating the analytical method(s) only. This analytical process would normally include repeating the analysis part of the method only with no additional sample preparative method(s) or cleanup method(s) being performed. A 'Reanalysis' typically involves taking another aliquot of the original sample through the entire analytical process. This analytical process would normally include applying the same preparative method(s), cleanup method(s) and analytical method(s) as were used during the analysis of the original sample. Or, it could involve simply performing another cleanup method to an already processed aliquot. A 'Dilution' involves taking a previously processed aliquot, performing a dilution and then repeating the analysis part of the method only with no additional sample preparative method(s) or cleanup method(s) being performed.

AnalysisGroup Client's identifier to define the type of AnalysisGroup.

DATA ELEMENT	DESCRIPTION

Analyst

Format: Text

Type:

Definition: The name or initials of the individual performing this task.

Applicable Node(s):

Handling

Analysis

PreparationPlusCleanup

Analyte

Format:

Type:

Definition: A parent data element that describes the analyte level data from one analysis or one group of analyses.

Applicable Node(s):

Analysis

AnalysisGroup

AnalyteComparison

Format:

Type:

Definition: A parent data element that describes data related to the comparison of two or more analytes such as those data elements that describe the effects of potentially interfering analytes on a peak.

Applicable Node(s):

Peak

DATA ELEMENT	DESCRIPTION

AnalyteGroup

Format:

Type:

Definition: A parent data element that links data associated with multiple measured analytes used to calculate results for another analyte.

Applicable Node(s):

Analysis

AnalysisGroup

AnalyteGroupID

Format: Identifier

Type: Required Conditionally

Definition: A laboratory-defined identifier that is used to link together multiple analytes to generate a single analyte result that is dependent upon each individual analyte.

Applicable Node(s):

AnalyteGroup	Analyte groups are used to link together analytes that are individually measured to report a different analyte as a final result. For example, an AnalyteGroup could be used to report a Hardness value that was determined by measuring individual Calcium and Magnesium values. An AnalyteGroup could also be used to report a total Xylene value that was determined by measuring the individual o-Xylene and p,m-Xylene values.
Analyte	The AnalyteGroup this analyte is part of.
ReportedResult	The AnalyteGroup this final result was derived from.

DATA ELEMENT	DESCRIPTION

AnalyteName

Format: Limited List

Type: Required for Portability

Definition: The published reference name of the analyte.

Applicable Node(s):

ReportedResult	If no published name is available then the ClientAnalyteName data element should be used. The published reference name could come from the Chemical Abstracts Service (CAS) 9th Collective Index Period (CIP), EPA's Chemical Registry Name, or some other published reference.
Analyte	
AnalyteComparison	AnalyteName for the analyte to compare to.
AnalyteGroup	AnalyteName for the analyte that belongs to this AnalyteGroup.
PeakComparison	AnalyteName for the analyte to compare to.

AnalyteNameContext

Format: Limited List

Type: Required for Portability

Definition: The published reference from which the AnalyteName is obtained.

Applicable Node(s):

ReportedResult

Analyte

AnalyteComparison

AnalyteGroup

PeakComparison

DATA ELEMENT	DESCRIPTION
AnalyteType	
Format: Limited List	
Type: Required	
Definition:	A term that identifies the type of analyte reported.
Applicable Node(s):	
ReportedResult	Example Valid Values: ‘Spike’ and ‘TIC’ (a non-routine analyte that is tentatively identified). For a routine method analyte, the default Valid Value is ‘Target.’
Analyte	Example Valid Values:‘Spike’, ‘TIC’ ‘Internal_Standard’, ‘Surrogate’, ‘System_Monitoring_Compound’, and ‘Tracer.’ For a routine method analyte, the default Valid Value is ‘Target.’
AnalyteGroup	
AnalyzedAmount	
Format: Numeric	
Type:	
Definition:	The amount (weight or volume) of a sample aliquot, prepared extract or standard that is used for an analysis.
Applicable Node(s):	
Analysis	If the analytical method requires the prior use of preparative or cleanup step(s), then the AnalyzedAmount is the actual amount of this final extract that is used for the analytical method. This would most often be used where a discrete measured sample aliquot, prepared extract or standard is introduced onto the instrument for analysis.
AnalyzedAmountUnits	
Format: Limited List	
Type:	
Definition:	Units for AnalyzedAmount.
Applicable Node(s):	
Analysis	

DATA ELEMENT	DESCRIPTION

AnalyzedDate

Format: Date

Type:

Definition: The date (and time, if required) of analysis of a sample aliquot or standard. If analyzed over a range of dates, this is the start date.

Applicable Node(s):

Analysis

AnalyzedEndDate

Format: Date

Type:

Definition: The date (and time, if required) of the end of the analysis period, if the sample aliquot or standard was analyzed over a period of time.

Applicable Node(s):

Analysis

ApparatusID

Format: Identifier

Type:

Definition: The laboratory-defined identifier for the analytical system used to process the sample or aliquot.

Applicable Node(s):

Analysis

Handling Example: An identifier for a TCLP device.

PreparationPlusCleanup Example: An identifier for a GPC or Purge-and-Trap device.

Autosampler

Format: Limited List

Type:

Definition: Indicates whether or not an autosampler was used.

Applicable Node(s):

Analysis Example Valid Values: ‘Yes’, ‘No.’

DATA ELEMENT	DESCRIPTION

BackgroundCorrection

Format: Limited list

Type:

Definition: Indicates whether or not background correction was done.

Applicable Node(s):

Analysis Example Valid Values: ‘Yes’, ‘No.’

BackgroundRawData

Format: Limited List

Type:

Definition: Indicates whether or not background raw data was generated when background correction was done.

Applicable Node(s):

Analysis Example Valid Values: ‘Yes’, ‘No.’

BackgroundType

Format: Limited List

Type:

Definition: The type of background correction performed during an analysis.

Applicable Node(s):

Analysis Example Valid Values: ‘Smith_Hieftje’, ‘Deuterium_Arc’, ‘Zeeman.’

Analyte Same as Analysis.

Peak Same as Analysis.

DATA ELEMENT	DESCRIPTION

BiasErrorRatio

Format: Numeric

Type:

Definition: The difference between the Result and ExpectedResult as a fraction of the square root of sum of squares of the ResultUncertainty and ExpectedResultUncertainty.

Applicable Node(s):

ReportedResult	For method QC of QCCategory Blank_Spike and Blank_Spike_Duplicate, the difference between the Result and ExpectedResult as a fraction of the square root of sum of squares of the ResultUncertainty and ExpectedResultUncertainty. For method QC of QCCategory Spike and Spike_Duplicate, the spiked Result minus the original Result and the ExpectedResult as a fraction of the square root of sum of squares of the ResultUncertainty of the Results and the ExpectedResultUncertainty.
Analyte	Same as in ReportedResult except applied to the results of analyses in an analysis group rather than a QC sample and original pair.
Peak	Same as in Analyte when results are measured per peak.

BillingID

Format: Identifier

Type:

Definition: A client-defined identifier to submit with the data for billing purposes.

Applicable Node(s):

SamplePlusMethod

BiologicalClassName

Format: Limited List

Type:

Definition: A broad classification of a sample organism.

Applicable Node(s):

SamplePlusMethod	Not necessarily intended to be the taxonomic class, but that is a possible value. Example Valid Values: ‘Animal’, ‘Commercial_Animal’, ‘Fish’, or ‘Plant.’

DATA ELEMENT	DESCRIPTION

Bottles

Format: Numeric

Type:

Definition: The number of containers received by the laboratory for this sample analysis.

Applicable Node(s):

SamplePlusMethod

BottleID

Format: Identifier

Type:

Definition: An identifier for the container that holds the sample being analyzed.

Applicable Node(s):

SamplePlusMethod

Analysis

Handling

PreparationPlusCleanup

BottleType

Format: Limited List

Type:

Definition: The size and type of container used to hold the sample.

Applicable Node(s):

SamplePlusMethod Example Valid Value: ‘1-L_Amber_Glass.’

DATA ELEMENT	DESCRIPTION

CalibrationBasis

Format: Limited List

Type:

Definition: The node (Analyte or Peak) that contains the calibration information for a given analyte.

Applicable Node(s):

Analyte

Example Valid Values:

1. When the calibration and subsequent quantitation for a given analyte is based on the use of a single peak when only a single peak is present, the valid value 'Peak' shall be used. All peak and calibration information shall be reported in the Peak node.
2. When the calibration and subsequent quantitation for a given analyte is based on the use of a single peak when multiple peaks are present, the valid value 'Peak' shall be used. All peak and calibration information shall be reported in the Peak node. In order to clearly indicate which peak of the multiple peaks was used for calibration, use the data element PeakID in the Analyte and ReportedResult nodes.
3. When the calibration for a given analyte is based on the use of multiple peaks with a unique calibration curve generated for each peak, the valid value 'Peak' shall be used. All peak and calibration information shall be reported in the Peak node. The method or project shall clearly indicate how each of the individually calculated peak results would be combined together to form the analyte result.
4. When the calibration and subsequent quantitation for a given analyte is based on combining two or more peaks, the valid value 'Analyte' shall be used. All calibration information shall be reported in the Analyte node and all individual peak information shall be reported in the Peak node. The method or project shall clearly indicate how each of the individual peak measurements would be combined to form the response that would be reported and used in the Analyte node to construct the calibration curve.
5. When the calibration and subsequent quantitation for a given analyte is not based on a peak (e.g., pH, conductivity), the valid value 'Analyte' shall be used. All calibration information shall be reported in the Analyte node.

DATA ELEMENT	DESCRIPTION

CalibrationFactor

Format: Numeric

Type:

Definition: The ratio of the detector response to the amount (mass or concentration) of analyte. It is a factor that is used to convert a detector response to an analyte result.

Applicable Node(s):

Analyte The calibration factor for this analyte.

Peak Same as in Analyte, except applied per peak.

CalibrationFactorUnits

Format: Text

Type:

Definition: Units for CalibrationFactor.

Applicable Node(s):

Analyte

Peak

CalibrationType

Format: Limited List

Type:

Definition: The calibration model used (for a particular analyte or peak) to define the initial calibration curve for a method.

Applicable Node(s):

Analyte The calibration type for this analyte. Example Valid Values: ‘Average_Relative_Response_Factor’, ‘Average_Calibration_Factor’, ‘Linear_Regression’, ‘Linear_Regression_With_Zero_Force’, ‘Quadratic_Regression’, ‘Quadratic_Regression_With_Zero_Force.’

Peak Same as in Analyte, except applied per peak.

DATA ELEMENT	DESCRIPTION

CASRegistryNumber

Format: Identifier

Type: Required for Portability

Definition:	The Chemical Abstract Service (CAS) registry number for the analyte.
Applicable Node(s):	
ReportedResult	This number would be represented using dashes between the three sets of numbers (e.g., 75-71-8).
Analyte	
AnalyteComparison	CASRegistryNumber for the analyte to compare to.
AnalyteGroup	CASRegistryNumber for the analyte that belongs to this AnalyteGroup.
PeakComparison	CASRegistryNumber for the analyte to compare to.

Characteristic

Format:

Type:

Definition:	A parent data element that identifies and quantifies the intrinsic characteristics associated with a sample as received by a laboratory or after the sample has been processed through a handling or preparation method.

Applicable Node(s):

Handling

PreparationPlusCleanup

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

CharacteristicType

Format: Limited List

Type: Conditionally Required

Definition: A term that identifies the type of characteristic being reported.

Applicable Node(s):

Handling	Characteristic of the sample after the handling described in this node.
PreparationPlusCleanup	Characteristic of the sample aliquot after the preparation or cleanup described in this node.
SamplePlusMethod	Characteristic of the sample as received.

CharacteristicUnits

Format: Limited List

Type:

Definition: Units for CharacteristicValue.

Applicable Node(s):

Handling

PreparationPlusCleanup

SamplePlusMethod

CharacteristicValue

Format: Text

Type:

Definition: A measured or observed value for the characteristic being reported. The value can either be numeric or text based on the characteristic being reported.

Applicable Node(s):

Handling	The measured or observed characteristic value after the handling described in this node.
PreparationPlusCleanup	The measured or observed characteristic value after the preparation or cleanup described in this node.
SamplePlusMethod	The measured or observed characteristic value of the sample as received.

DATA ELEMENT	DESCRIPTION

Checksum

Format: Numeric

Type:

Definition: A value based on all other data in a node that can be used to check the integrity of an electronic data deliverable.

Applicable Node(s):

All This field can be used in any node. Its value applies to the node it is in. The required algorithm to compute the data for this field is as follows: For all data in a node, starting with the first data element line, ending before the next node or end of the data stream, and ignoring 1) The carriage return and linefeed at the end of each line. 2) Any optional leading spaces in data element lines. 3) The entire line with the checksum field. Compute the sum of the ASCII codes of all non-ignored characters. Report this sum as an integer.

CleanedUpDate

Format: Date

Type:

Definition: The date (and time, if required) of any cleanup procedure performed on the sample aliquot. If cleaned up over a range of dates, this is the start date.

Applicable Node(s):

PreparationPlusCleanup

CleanedUpEndDate

Format: Date

Type:

Definition: The date (and time, if required), of the end of the cleanup period, if the sample aliquot was cleaned up over a period of time.

Applicable Node(s):

PreparationPlusCleanup

DATA ELEMENT	DESCRIPTION
CleanupBatch	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier that is used to link multiple sample aliquots that are cleaned up together for processing by one method. "Together" implies similarity of time, place, and manner of cleanup.
Applicable Node(s):	
PreparationPlusCleanup	The definition of a cleanup batch depends on the method but might be linked to cleanup specific QC samples.
CleanupID	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier for this cleanup event for this aliquot.
Applicable Node(s):	
PreparationPlusCleanup	
CleanupType	
Format: Text	
Type:	
Definition:	A term that identifies the specific cleanup performed when multiple options are given within the referenced method.
Applicable Node(s):	
PreparationPlusCleanup	This term is used to specify which cleanup method was used when such cleanup method details are part of the analysis (instrumental) method. When client cleanup methods are available, this term can be used to identify what method options were used within the cleanup method.
InstrumentQC	For Instrument QC with QCLinkage 'CleanupBatch', a term that identifies the type of cleanup this QC pertains to. The field's value must match that specified as the CleanupType for cleanups of associated samples.

DATA ELEMENT	DESCRIPTION
ClientAnalysisID	
Format: Identifier	
Type:	
Definition:	A client-defined identifier for an analysis.
Applicable Node(s):	
Analysis	
ClientAnalyteID	
Format: Identifier	
Type: Required	
Definition:	A client-defined identifier for an analyte.
Applicable Node(s):	
ReportedResult	
Analyte	
AnalyteComparison	ClientAnalyteID for the analyte to compare to.
AnalyteGroup	ClientAnalyteID for the analyte that belongs to this AnalyteGroup.
PeakComparison	ClientAnalyteID for the analyte to compare to. If not specified, it is assumed to be the same as the analyte for the Peak element this PeakComparison element is in.
ClientAnalyteName	
Format: Text	
Type:	
Definition:	A client-defined common name for an analyte.
Applicable Node(s):	
ReportedResult	
Analyte	
AnalyteComparison	ClientAnalyteName for the analyte to compare to.
AnalyteGroup	ClientAnalyteName for the analyte that belongs to this AnalyteGroup.
PeakComparison	ClientAnalyteName for the analyte to compare to.

DATA ELEMENT	DESCRIPTION

ClientDetectionLimit

Format: Numeric

Type:

Definition: A client-specified upper limit of the detection limit of the analyte being measured.

Applicable Node(s):

ReportedResult Depending on client and method specific rules, required detection limits might be scaled by factors such as dilution and percent moisture prior to reporting.

Analyte

Peak

ClientDetectionLimitUnits

Format: Limited List

Type:

Definition: Units for ClientDetectionLimit.

Applicable Node(s):

ReportedResult If the client specifies that the ClientDetectionLimitUnits must be the same as the ResultUnits, the ClientDetectionLimitUnits need not be specified.

Analyte Same as in ReportedResult.

Peak Same as in ReportedResult.

ClientID

Format: Identifier

Type:

Definition: An client-defined identifier for the person or organization ordering the analysis of these samples. Different clients will often have different reporting and Quality Assurance/Quality Control (QA/QC) requirements. To be fully reliable, this identifier must be unique across all potential clients to allow one client to read the data as reported in this data package by another client.

Applicable Node(s):

Header

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

ClientInstrumentQCType

Format: Limited List

Type:

Definition: A client-defined designation used to define how a given Instrument Quality Control (QC) sample(s) was implemented.

Applicable Node(s):

InstrumentQC For example, whether one, two or more mixes were used to perform an initial calibration or a continuing calibration verification.

ClientMethodCategory

Format: Text

Type:

Definition: The client-defined general class or common name for the group of analytes being measured by a given method for this sample.

Applicable Node(s):

SamplePlusMethod Examples: VOAs, SVOAs, Metals, PCBs, PESTs.

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

ClientMethodCode

Format: Text

Type:

Definition: A client-defined code for the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

ClientMethodID

Format: Identifier

Type: Required

Definition: A client-defined identifier for the method used by the laboratory to analyze the sample.

Applicable Node(s):

- **SamplePlusMethod** — This identifier usually consists of numbers or a combination of letters and numbers.
- **InstrumentQC**
- **Handling**
- **PreparationPlusCleanup**
- **Analysis**

ClientMethodModificationDescription

Format: Text

Type:

Definition: Text that describes any modifications made to the client's method.

Applicable Node(s):

- **SamplePlusMethod**
- **InstrumentQC**
- **Handling**
- **PreparationPlusCleanup**
- **Analysis**

DATA ELEMENT	DESCRIPTION

ClientMethodModificationID

Format: Identifier

Type:

Definition: A client-defined identifier that identifies modifications made to the client's method.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

ClientMethodName

Format: Text

Type:

Definition: A client-defined method name or title of the analysis method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

ClientMethodSource

Format: Text

Type:

Definition: The author or publishing agency of the ClientMethodID and ClientMethodName.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

ClientMethodType

Format: Text

Type:

Definition: The method classification or technology of the ClientMethodID and ClientMethodName.

Applicable Node(s):

SamplePlusMethod The type of technology being used to analyze this sample. Example: GC/MS, GC/MS_SIM, ICP/AES, IR.

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

ClientMethodVersion

Format: Text

Type:

Definition: The revision or version of the ClientMethodID and ClientMethodName.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

ClientName

Format: Text

Type:

Definition: The person or organization ordering the analysis of these sample(s).

Applicable Node(s):

Header

SamplePlusMethod

ClientQuantitationLimit

Format: Numeric

Type:

Definition: A client-specified upper limit of the quantitation limit of the analyte being measured.

Applicable Node(s):

ReportedResult Depending on client and method specific rules, required quantitation limits might be scaled by factors such as dilution and percent moisture prior to reporting.

Analyte

Peak

DATA ELEMENT	DESCRIPTION

ClientQuantitationLimitUnits

Format: Limited List

Type:

Definition: Units for ClientQuantitationLimit.

Applicable Node(s):

ReportedResult	If the client specifies that the ClientQuantitationLimitUnits must be the same as the ResultUnits, the ClientQuantitationLimitUnits need not be specified.
Analyte	Same as in ReportedResult.
Peak	Same as in ReportedResult.

ClientSampleID

Format: Identifier

Type: Required

Definition: A client-defined identifier that uniquely identifies a single sample that is subjected to an analysis.

Applicable Node(s):

SamplePlusMethod	This should be the basis on which the client identifies the sample. However, not all clients define values for laboratory-generated QC samples.

Coeffa0

Format: Numeric

Type:

Definition: The value of the zeroth order coefficient in a polynomial or regression equation. This term is sometimes referred to as the ‘b’ value or ‘y-intercept’ for a linear regression.

Applicable Node(s):

Analyte

Peak

DATA ELEMENT	DESCRIPTION
Coeffa1	
Format: Numeric	
Type:	
Definition:	The value of the first order coefficient in a polynomial or regression equation. This term is sometimes referred to as the 'slope' for a linear regression.
Applicable Node(s):	
Analyte	Used for an analyte in AnalysisGroup.
Peak	Same as in Analyte, except applied per peak.
Coeffa2	
Format: Numeric	
Type:	
Definition:	The value of the second order coefficient in a polynomial equation. This element would be reported if using a quadratic fit.
Applicable Node(s):	
Analyte	Used for an analyte in AnalysisGroup.
Peak	Same as in Analyte, except applied per peak.
Coeffa3	
Format: Numeric	
Type:	
Definition:	The value of the third order coefficient in a polynomial equation.
Applicable Node(s):	
Analyte	Used for an analyte in AnalysisGroup.
Peak	Same as in Analyte, except applied per peak.

DATA ELEMENT	DESCRIPTION

CoeffOfDetermination

Format: Numeric

Type:

Definition: The Coefficient of Determination, typically expressed as R^2, is the proportion of variability in a data set that is accounted for by a statistical model. There is no consensus about the exact definition of R^2; however, it is generally referred to as the goodness of fit for a polynomial equation.

Applicable Node(s):

Analyte Used for an analyte in AnalysisGroup.

Peak Same as in Analyte, except applied per peak.

CoeffOfDeterminationLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the CoeffOfDetermination.

Applicable Node(s):

Analyte

Peak

CoeffOfDeterminationLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the CoeffOfDetermination limits. Values reported within these limits indicate if the stated or expected data quality objectives for CoeffOfDetermination were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

DATA ELEMENT	DESCRIPTION

CollectedDate

Format: Date

Type:

Definition: The date (and time, if required) the sample was collected. If the sample was collected over a range of dates, this is the start date.

Applicable Node(s):

SamplePlusMethod

CollectedEndDate

Format: Date

Type:

Definition: The date (and time, if required), of the end of the sample collection period, if the sample was collected over a period of time.

Applicable Node(s):

SamplePlusMethod

Column

Format: Text

Type:

Definition: The name or type of the column or cartridge used by this method.

Applicable Node(s):

Analysis

PreparationPlusCleanup

ColumnInternalDiameter

Format: Numeric

Type:

Definition: The internal diameter of the column or cartridge.

Applicable Node(s):

Analysis

PreparationPlusCleanup

DATA ELEMENT	DESCRIPTION

ColumnInternalDiameterUnits

Format: Limited List

Type:

Definition: Units for ColumnInternalDiameter.

Applicable Node(s):

Analysis

PreparationPlusCleanup

ColumnLength

Format: Numeric

Type:

Definition: The length of the column or cartridge used by this method.

Applicable Node(s):

Analysis

PreparationPlusCleanup

ColumnLengthUnits

Format: Limited List

Type:

Definition: Units for ColumnLength.

Applicable Node(s):

Analysis

PreparationPlusCleanup

Comment

Format: Text

Type:

Definition: A free-form remark, observation, explanation, or expansion text that can occur in any parent data element.

Applicable Node(s):

All Its value applies to the data in the node it is in. Readers are not required to take any action based on these comments, but they may choose to record them as text comments in their database.

DATA ELEMENT	DESCRIPTION

Composite

Format: Limited List

Type:

Definition: Indicates whether or not the sample as received by the laboratory is a composite.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Yes’, ‘No.’

ConfirmationAnalysisID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for an analysis that confirms the results of this analysis. Final results are usually reported for a method from the primary analysis.

Applicable Node(s):

Analysis The LabAnalysisID for the confirmation analysis.

AnalysisGroup Same as Analysis except confirming results from this AnalysisGroup.

ContactInformation

Format:

Type:

Definition: A parent data element that describes the name, address and other contact information for the laboratory.

Applicable Node(s):

Header

CoolerID

Format: Identifier

Type:

Definition: A client-defined unique identifier for the cooler or other shipping container used to transport the sample to the laboratory.

Applicable Node(s):

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

CorrectionFactor

Format: Numeric

Type:

Definition: The correction factor for this peak, based on interanalyte effects from the analyte named in this node.

Applicable Node(s):

AnalyteComparison

CorrelationCoeff

Format: Numeric

Type:

Definition: The correlation coefficient, typically expressed as *r*, which measures the strength and direction of a linear relationship between two variables. The correlation coefficient is often used in linear regression to evaluate the goodness of fit of a given data set to a straight line.

Applicable Node(s):

Analyte Used for an analyte in AnalysisGroup such as might be determined from the method of standard additions or from an initial calibration.

Peak Same as in Analyte, except applied per peak.

CorrelationCoeffLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the CorrelationCoeff.

Applicable Node(s):

Analyte

Peak

DATA ELEMENT	DESCRIPTION

CorrelationCoeffLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the CorrelationCoeff limits. Values reported within these limits indicate if the stated or expected data quality objectives for CorrelationCoeff were achieved.

Applicable Node(s):

Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	

Counts

Format: Numeric

Type:

Definition: The number of disintegrations or particles counted by the detector during the analysis of the sample aliquot. This data element is normally used in radiochemical analyses.

Applicable Node(s):

Analysis	The Counts as measured by the detector during the analysis of the sample aliquot.
Analyte	Same as in Analysis when Counts are measured per analyte.
Peak	Same as in Analyte when Counts are measured per peak.

CountsUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the Counts, by which the Counts may differ from the true value during this analysis process.

Applicable Node(s):

Analysis	Expressed as an offset to the Counts (y) in the form: Counts ± positive numeric value ($y \pm a$).
Analyte	Same as in Analysis when Counts are measured per analyte.
Peak	Same as in Analyte when Counts are measured per peak.

DATA ELEMENT	DESCRIPTION

CountsUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, at which the CountsUncertainty was determined.

Applicable Node(s):

Analysis Reported as a value between 0 and 100%.

Analyte

Peak

CountsUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported CountsUncertainty.

Applicable Node(s):

Analysis This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality) should also be included; statistical experimental design (e.g., number of replicate measurements).

Analyte

Peak

CountsUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the Counts.

Applicable Node(s):

Analysis Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the Counts, ‘Other_Interval’ when the interval is not centered on the Counts.

Analyte

Peak

DATA ELEMENT	DESCRIPTION

CountsUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the Counts may differ from the true value due to this analysis process.

Applicable Node(s):

Analysis Expressed as a upper limit to the Counts in the form: Counts (y) < Upper Counts limit (a_H). When both Upper and Lower Counts limits are reported, the Counts should appear as: Lower Limit Counts (a_L) < Counts (y) < Upper Limit Counts (a_H).

Analyte Same as in Analysis when Counts are measured per analyte.

Peak Same as in Analyte when Counts are measured per peak.

CountsUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the Counts may differ from the true value due to this analysis process.

Applicable Node(s):

Analysis Expressed as a lower limit to the Counts in the form: Lower Counts limit (a_L) < Counts (y). When both Upper and Lower Counts limits are reported, the Counts should appear as: Lower Limit Counts (a_L) < Counts (y) < Upper Limit Counts (a_H).

Analyte Same as in Analysis when Counts are measured per analyte.

Peak Same as in Analyte when Counts are measured per peak.

DATA ELEMENT	DESCRIPTION

CountsUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the CountsUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

Analysis Example Valid Values: ‘Category A’ where the estimate of the CountsUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the CountsUncertainty is determined using some other method (in whole or in part).

Analyte

Peak

CountsUncertaintyUnits

Format: Limited List

Type:

Definition: Units for CountsUncertainty.

Applicable Node(s):

Analysis If the client specifies that the CountsUncertaintyUnits must be the same as the CountsUnits, the CountsUncertaintyUnits need not be specified.

Analyte

Peak

CountsUnits

Format: Limited List

Type:

Definition: Units for Counts.

Applicable Node(s):

Analysis

Analyte

Peak

DATA ELEMENT	DESCRIPTION
CreatedDate	
Format: Date	
Type:	
Definition:	The date (and time, if required) a Quality Control (QC) sample was generated or derived in the laboratory.
Applicable Node(s):	
SamplePlusMethod	
CustodyID	
Format: Identifier	
Type:	
Definition:	A client-defined identifier for the chain of custody document and/or tracking record associated with receipt of this sample in the laboratory.
Applicable Node(s):	
SamplePlusMethod	
DateFormat	
Format: Limited List	
Type:	
Definition:	A value that specifies the format of all reported date/time values in an electronic data deliverable. This value can incorporate the time zone, if required.
Applicable Node(s):	
Header	A required DateFormat value may be specified by the client or implementation.

DATA ELEMENT	DESCRIPTION
DetectionLimit	
Format: Numeric	
Type:	
Definition:	The detection limit of the analyte being measured. Detection limits are defined in terms of the presence or absence of the analyte within a stated confidence limit.
Applicable Node(s):	
ReportedResult	
Analyte	Within AnalysisGroup, applies to a detection limit value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
DetectionLimitType	
Format: Limited List	
Type:	
Definition:	A term that identifies the means by which the detection limit was determined or reported.
Applicable Node(s):	
ReportedResult	Example Valid Values: ‘CRDL’, ‘MDL’, ‘IDL.’
Analyte	
Peak	
DetectionLimitUnits	
Format: Limited List	
Type:	
Definition:	Units for DetectionLimit.
Applicable Node(s):	
ReportedResult	
Analyte	
Peak	

DATA ELEMENT	DESCRIPTION
DetectorID	
Format: Identifier	
Type:	
Definition:	A laboratory-defined unique identifier for a specific detector.
Applicable Node(s):	
Analysis	
DetectorType	
Format: Limited List	
Type:	
Definition:	The type of detector used in the instrumental analysis.
Applicable Node(s):	
Analysis	Example Valid Values: ‘FID’, ‘MS.’
DifferenceErrorRatio	
Format: Numeric	
Type:	
Definition:	The estimated error between two results defined as the absolute value of the difference of two values as a fraction of the square root of sum of squares of their ResultUncertainties.
Applicable Node(s):	
ReportedResult	Used with method QC of QCCategory Duplicate, Serial_Dilution, Spike_Duplicate, and Blank_Spike_Duplicate.
Analyte	Same as in ReportedResult except applied to the results of analyses in an analysis group rather than a QC sample and original pair.
Peak	Same as in Analyte when results are measured per peak.

DATA ELEMENT	DESCRIPTION
DilutionFactor	
Format: Numeric	
Type:	
Definition:	The overall dilution of the sample aliquot for a particular analysis. A value of one corresponds to nominal conditions for the method. Values greater than one correspond to dilutions. Values less than one correspond to concentrations.
Applicable Node(s):	
Analysis	Exactly which factors are included in the DilutionFactor may depend on the method. The most common useage involves dilution of a prepared extract immediately prior to analysis. Under these conditions the initial sample weight or volume would not normally be taken into account unless the sample were to be directly introduced into the instrument.
Drift	
Format: Numeric	
Type:	
Definition:	The difference between the actual location of a peak and its predicted position.
Applicable Node(s):	
Analysis	Example: For alpha spectroscopy, Drift is computed using the tracer peak.
Analyte	Same except applied to a specific analyte.
Peak	Same except applied to a specific peak.
DriftUnits	
Format: Limited List	
Type:	
Definition:	Units for Drift.
Applicable Node(s):	
Analysis	
Analyte	
Peak	

DATA ELEMENT	DESCRIPTION
EDDID	
Format: Limited List	
Type: Required	
Definition:	An identifier that specifies the format of an electronic data deliverable.
Applicable Node(s):	
Header	Must have the value 'SEDD'. It can be checked by readers to determine that following data are in a SEDD compatible format. Since this field need not be the first line in Header, readers need to be prepared to read all the Header lines before making this check.
EDDImplementationID	
Format: Limited List	
Type: Required	
Definition:	A identifier that identifies the specific implementation (Document Type Definition or Schema) of an electronic data deliverable.
Applicable Node(s):	
Header	A value specified in a SEDD implementation document (DTD or Schema) as the identifier of the implementation. This value should be checked by readers to determine that following data are in a processible format. For example, an implementation might specify what data elements are required in the EDD, including any implementation defined fields. Since this field need not be the first line in Header, readers need to be prepared to read all the fields in Header before checking this value.

DATA ELEMENT	DESCRIPTION

EDDImplementationVersion

Format: Limited List

Type: Required

Definition: A value that identifies the version of the specific implementation (Document Type Definition or Schema) of an electronic data deliverable.

Applicable Node(s):

Header A value specified in each revision of a SEDD implementation document (DTD or Schema). The value in an EDD indicates the version of the implementation that following data is compatible with. Reader programs may have to adapt their behavior based on this value. In particular, the list of implementation defined fields may change with version number. Implementors should assign version numbers so that later versions have later alphanumeric version numbers.

EDDVersion

Format: Limited List

Type: Required

Definition: A value that specifies the version of the format of an electronic data deliverable.

Applicable Node(s):

Header Specified in each revision of the SEDD Specification. Specified by the writer of an EDD to indicate the version of SEDD that following data is compatible with. Reader programs may have to adapt their behavior based on this value. In particular, the list of SEDD defined fields may change with version number.

DATA ELEMENT	DESCRIPTION

Efficiency

Format: Numeric

Type: Required

Definition: The Efficiency of the instrument as a percent. Usually used in radiochemistry to mean the counts detected as a percentage of the decays actually occurring.

Applicable Node(s):

Analysis	
Analyte	Efficiency as applied to a specific analyte.
Peak	Efficiency as applied to a specific analyte and peak.
PreparationPlusCleanup	Efficiency of the Preparation or Cleanup process that relates to the percent of the original material actually processed by this preparation or cleanup procedure.

Energy

Format: Numeric

Type:

Definition: The energy of an emission.

Applicable Node(s):

Peak	For example, decay energy as used in radiochemistry.
PeakComparison	

EnergyUnits

Format: Limited List

Type:

Definition: Units for Energy.

Applicable Node(s):

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION
EquipmentBatch	
Format: Identifier	
Type:	
Definition:	An identifier that is used to link multiple samples collected using the same equipment in a defined period of time. Operationally, this batch associates a field equipment blank with a group of samples.
Applicable Node(s):	
SamplePlusMethod	This value is currently often not known to the laboratory. It might be merged with laboratory data by a validator.
ExpectedResult	
Format: Numeric	
Type:	
Definition:	The expected or theoretical result of an analyte that has been spiked into a sample aliquot or a standard at any time during the analysis process. The true value of an analyte in the sample analyzed or the expected or theoretical result of a purchased or prepared standard.
Applicable Node(s):	
ReportedResult	Specifies the expected or theoretical result of analyte that has been spiked into the sample aliquot or standard. For these spiked samples, the expected or theoretical result would be determined only from the amount of analyte spiked and would not include any native analyte concentrations that might have been present in the original sample. Can also specify the actual true value of an analyte in a sample, such as would be the case for a Standard Reference Material (SRM).
Analyte	Same as in the ReportedResult node extended so ExpectedResult can now refer to spikes, surrogates, internal standards, tracers and standard additions where known amounts have been added to samples or standards for QC purposes. This can also represent the expected or theoretical result of an analyte in a purchased or prepared standard.

DATA ELEMENT	DESCRIPTION

ExpectedResultUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the ExpectedResult, by which the ExpectedResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s):

ReportedResult Expressed as an offset to the ExpectedResult (y) in the form: ExpectedResult ± positive numeric value ($y \pm a$).

Analyte Extended to anything considered to be the Expected Result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.

ExpectedResultUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, at which the ExpectedResultUncertainty was determined.

Applicable Node(s):

ReportedResult Reported as a value between 0 and 100%.

Analyte

ExpectedResultUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported ExpectedResultUncertainty.

Applicable Node(s):

ReportedResult This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality) should also be included; statistical experimental design (e.g., number of replicate measurements).

Analyte

DATA ELEMENT	DESCRIPTION

ExpectedResultUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the ExpectedResult.

Applicable Node(s):

ReportedResult Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the ExpectedResult, ‘Other_Interval’ when the interval is not centered on the ExpectedResult.

Analyte

ExpectedResultUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the ExpectedResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s)

ReportedResult Expressed as a upper limit to the ExpectedResult in the form: ExpectedResult (y) < Upper ExpectedResult limit (a_H). When both Upper and Lower ExpectedResult limits are reported, the ExpectedResult should appear as: Lower Limit ExpectedResult (a_L) < ExpectedResult (y) < Upper Limit ExpectedResult (a_H).

Analyte Extended to anything considered to be the ExpectedResult of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.

DATA ELEMENT	DESCRIPTION

ExpectedResultUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the ExpectedResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s):

ReportedResult Expressed as a lower limit to the ExpectedResult in the form: Lower ExpectedResult limit (a_L) < ExpectedResult (y). When both Upper and Lower ExpectedResult limits are reported, the ExpectedResult should appear as: Lower Limit ExpectedResult (a_L) < ExpectedResult (y) < Upper Limit ExpectedResult (a_H).

Analyte Extended to anything considered to be the ExpectedResult of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.

ExpectedResultUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the ExpectedResultUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

ReportedResult Example Valid Values: ‘Category A’ where the estimate of the ExpectedResultUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the ExpectedResultUncertainty is determined using some other method (in whole or in part).

Analyte

DATA ELEMENT	DESCRIPTION

ExpectedResultUncertaintyUnits

Format: Limited List

Type:

Definition: Units for ExpectedResultUncertainty.

Applicable Node(s):

ReportedResult

Analyte

ExpectedResultUnits

Format: Limited List

Type:

Definition: Units for ExpectedResult.

Applicable Node(s):

ReportedResult

Analyte

FieldSampleID

Format: Identifier

Type:

Definition: A sampler-defined identifier assigned to a sample. This identifier is not assigned by the client.

Applicable Node(s):

SamplePlusMethod This value is often not known to the laboratory. It could be useful as a link into the sampling records system.

Filtered

Format: Limited List

Type:

Definition: Indicates whether or not the sample as received by the laboratory was field filtered.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Yes’, ‘No.’

DATA ELEMENT	DESCRIPTION

FilterSize

Format: Numeric

Type:

Definition: The filter pore size for samples, aliquots or extracts that are filtered.

Applicable Node(s):

SamplePlusMethod

Handling

Analysis

PreparationPlusCleanup

FilterSizeUnits

Format: LimitedList

Type:

Definition: Units for FilterSize.

Applicable Node(s):

SamplePlusMethod

Handling

Analysis

PreparationPlusCleanup

FinalAmount

Format: Numeric

Type:

Definition: The amount (weight or volume) of material (i.e., digestate, extract, distillate, etc.) generated as the outcome of processing a sample aliquot through a single sample preparation or cleanup process.

Applicable Node(s):

Analysis

PreparationPlusCleanup

DATA ELEMENT	DESCRIPTION

FinalAmountUnits

Format: Limited List

Type:

Definition: Units for FinalAmount.

Applicable Node(s):

Analysis

PreparationPlusCleanup

FlowRate

Format: Numeric

Type:

Definition: The rate of flow of a gas or liquid mobile phase as often used in chromatography.

Applicable Node(s):

Analysis

FlowRateUnits

Format: Limited List

Type:

Definition: Units for FlowRate.

Applicable Node(s):

Analysis

Frequency

Format: Numeric

Type:

Definition: The frequency of an emission or absorption.

Applicable Node(s):

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION

FrequencyUnits

Format: Limited List

Type:

Definition: Units for Frequency.

Applicable Node(s):

Peak

PeakComparison

GeneratingSystemID

Format: Identifier

Type:

Definition: A laboratory-defined identifier that names the software system used to generate an electronic data deliverable. This identifier may be built into commercial software.

Applicable Node(s):

Header The reader may use this value to adapt to known quirks of the generating system.

GeneratingSystemVersion

Format: Text

Type:

Definition: A laboratory-defined version number of the software system used to generate an electronic data deliverable.

Applicable Node(s):

Header

Gradient

Format: Numeric

Type:

Definition: The temperature gradient for z gas chromatograph or the mobile phase gradient for a high performance liquid chromatograph.

Applicable Node(s):

Analysis

DATA ELEMENT	DESCRIPTION

GradientUnits

Format: Limited List

Type:

Definition: Units for Gradient.

Applicable Node(s):

Analysis

HandledDate

Format: Date

Type:

Definition: The date (and time, if required) of handling of this sample. If handled over a range of dates, this is the start date.

Applicable Node(s):

Handling

HandledEndDate

Format: Date

Type:

Definition: The date (and time, if required) of the end of the handling period of the sample, if the sample was handled over a period of time.

Applicable Node(s):

Handling

Handling

Format:

Type:

Definition: A parent data element that describes any manipulation of the sample (e.g., leaching, filtering, ashing) prior to taking a sample aliquot for analysis.

Applicable Node(s)

SamplePlusMethod

DATA ELEMENT	DESCRIPTION
HandlingBatch	
Format: Identifier	
Type:	
Definition:	An identifier that is used to link multiple samples that are handled together. Together can imply similarity of time, place, and manner of handling.
Applicable Node(s):	
Handling	The definition of a handling batch depends on the method but might be linked to handling specific Quality Control (QC) samples. Example: All samples associated with one TCLP apparatus blank would be in one HandlingBatch of ClientMethodID 1311. The method QC sample in the batch might have QCType TCLP_Blank.
HandlingDuration	
Format: Numeric	
Type:	
Definition:	The duration of the handling process performed on a sample.
Applicable Node(s):	
Handling	Example: TCLP leaching time.
HandlingDurationUnits	
Format: Limited List	
Type:	
Definition:	Units for HandlingDuration.
Applicable Node(s):	
Handling	

DATA ELEMENT	DESCRIPTION
HandlingFactor	
Format: Numeric	
Type:	
Definition:	A factor that reflects processing done early in sample handling.
Applicable Node(s):	
Handling	For example, used in radiochemistry with a hot laboratory that does preliminary processing prior to more routine activities.
HandlingFactorUnits	
Format: Limited List	
Type:	
Definition:	Units for HandlingFactor.
Applicable Node(s):	
Handling	
HandlingID	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier for this handling event for this sample.
Applicable Node(s):	
Handling	

DATA ELEMENT	DESCRIPTION
HandlingType	
Format: Text	
Type:	
Definition:	A client-defined term that identifies the specific type of preliminary processing done to a sample, prior to aliquotting, when multiple options are given within the referenced method or when no referenced method is available.
Applicable Node(s):	
Handling	This description is used to specify which handling method was used when such handling method details are part of the analysis (instrumental) method. When client cleanup method codes are available, this description is used to identify what method options were used within the handling method.
SamplePlusMethod	For a method QC sample with QCLinkage 'HandlingBatch', a code that identifies the type of handling this QC pertains to. The field's value must match that specified as the HandlingType for handlings of associated samples.
Header	
Format:	
Type:	
Definition:	A parent data element that describes the format and content of the electronic data deliverable.
Applicable Node(s):	
HeatedPurge	
Format: Limited List	
Type:	
Definition:	Indicates whether or not a heated purge was used for volatiles analysis.
Applicable Node(s):	
Analysis	Example Valid Values: 'Yes', 'No.'

DATA ELEMENT	DESCRIPTION

Inclusion

Format: Limited List

Type:

Definition: Indicates whether or not this item is to be included and evaluated as part of this data package.

Applicable Node(s):

Analysis	Whether or not this analysis is to be included and evaluated as part of this data package. An analysis may not be included if it failed to meet project requirements and another analysis had been completed that was meant to replace the original one. Example Valid Values: 'Yes', 'No.'
Analyte	Whether or not this analyte is to be included and evaluated as part of this data package. An analyte may not be included in an Initial Calibration sequence if its response does not meet minimum project requirements.
Peak	Whether or not this peak is to be included and evaluated as part of this data package. A peak may not be included if its response has been affected by interferences.

InitialAmount

Format: Numeric

Type:

Definition: The amount (weight or volume) of material used for processing the sample through a single handling or cleanup process.

Applicable Node(s):

Handling	The amount of material used for this handling method.
PreparationPlusCleanup	For a cleanup process, the amount of material used for this cleanup method. For a preparation process, the amount of solvent used that the sample analytes will be transferred to, such as might be used for medium-level soil analysis for Volatile Organics where an initial amount of methanol is added to the original sample aliquot.

DATA ELEMENT	DESCRIPTION

InitialAmountUnits

Format: Limited List

Type:

Definition: Units for InitialAmount.

Applicable Node(s):

Handling

PreparationPlusCleanup

InjectionVolume

Format: Numeric

Type:

Definition: The volume of sample injected/purged into the instrument or onto a specific column when an injection is split between two or more columns.

Applicable Node(s):

Analysis

InjectionVolumeUnits

Format: Limited List

Type:

Definition: Units for InjectionVolume.

Applicable Node(s):

Analysis

InstrumentID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for an instrument.

Applicable Node(s):

Analysis

DATA ELEMENT	DESCRIPTION

InstrumentQC

Format:

Type:

Definition: A parent data element related to instrument or process quality control data (e.g., initial and continuing calibration).

Applicable Node(s):

Header

InstrumentSerialNumber

Format: Text

Type:

Definition: The serial number of the instrument used for this analysis.

Applicable Node(s):

Analysis

InterelementCorrection

Format: Limited List

Type:

Definition: Indicates whether or not Inductively Coupled Plasma (ICP) interelement or interanalyte correction factors were applied.

Applicable Node(s):

Analysis Example Valid Values: ‘Yes’, ‘No.’

IntermediateResult

Format: Numeric

Type:

Definition: The results of this analysis, not for a method, and would normally not include sample aliquot, dilution or other sample information. This value is normally the result obtained directly from a calibration curve.

Applicable Node(s):

Analyte The result for this analyte for an analysis, not a method.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

DATA ELEMENT	DESCRIPTION

IntermediateResultLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the IntermediateResult.

Applicable Node(s):

Analyte This would typically represent the upper limit of the calibrated range for this analyte.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

IntermediateResultLimitLow

Format: Numeric

Type:

Definition: The lowerest boundary or limit used for the IntermediateResult.

Applicable Node(s):

Analyte This would typically represent the lower limit of the calibrated range for this analyte.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

IntermediateResultLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the IntermediateResult limits. Values reported within these limits indicate if the stated or expected data quality objectives for IntermediateResult were achieved.

Applicable Node(s):

Analyte

Peak

PeakReplicate

DATA ELEMENT	DESCRIPTION

IntermediateResultUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the IntermediateResult, by which the IntermediateResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s):

Analyte	Expressed as an offset to the IntermediateResult (*y*) in the form: IntermediateResult ± positive numeric value ($y \pm a$). Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

IntermediateResultUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, that the IntermediateResultUncertainty was determined at.

Applicable Node(s):

Analyte	Reported as a value between 0 and 100%.
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION

IntermediateResultUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported IntermediateResultUncertainty.

Applicable Node(s):

Analyte This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality); statistical experimental design (e.g., number of replicate measurements).

Peak

PeakReplicate

IntermediateResultUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the IntermediateResult.

Applicable Node(s):

Analyte Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the IntermediateResult, ‘Other_Interval’ when the interval is not centered on the IntermediateResult.

Peak

PeakReplicate

DATA ELEMENT	DESCRIPTION

IntermediateResultUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the IntermediateResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s):

Analyte Expressed as a upper limit to the IntermediateResult in the form: IntermediateResult (y) < Upper IntermediateResult limit (a_H). When both Upper and Lower IntermediateResult limits are reported, the IntermediateResult should appear as: Lower Limit IntermediateResult (a_L) < IntermediateResult (y) < Upper Limit IntermediateResult (a_H). Within AnalysisGroup, applies to a mean or other value computed from several analyses.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

IntermediateResultUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the IntermediateResult may differ from the true value due to all effects related to analysis by the laboratory.

Applicable Node(s):

Analyte Expressed as a lower limit to the IntermediateResult in the form: Lower IntermediateResult limit (a_L) < IntermediateResult (y). When both Upper and Lower IntermediateResult limits are reported, the IntermediateResult should appear as: Lower Limit IntermediateResult (a_L) < IntermediateResult (y) < Upper Limit IntermediateResult (a_H). Within AnalysisGroup, applies to a mean or other value computed from several analyses.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

DATA ELEMENT	DESCRIPTION

IntermediateResultUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the IntermediateResultUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

Analyte Example Valid Values: ‘Category A’ where the estimate of the IntermediateResultUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the IntermediateResultUncertainty is determined using some other method (in whole or in part).

Peak

PeakReplicate

IntermediateResultUncertaintyUnits

Format: Limited List

Type:

Definition: Units for IntermediateResultUncertainty.

Applicable Node(s):

Analyte If the client specifies that the IntermediateResultUncertaintyUnits must be the same as the IntermediateResultUnits, the IntermediateResultUncertaintyUnits need not be specified.

Peak Same as in Analyte, when results are measured per peak.

PeakReplicate

DATA ELEMENT	DESCRIPTION

IntermediateResultUnits

Format: Limited List

Type:

Definition: Units for IntermediateResult.

Applicable Node(s):

Analyte

Peak

PeakReplicate

LabAddress1

Format: Text

Type:

Definition: The primary street address of the location of the laboratory performing this analysis.

Applicable Node(s):

ContactInformation

LabAddress2

Format: Text

Type:

Definition: The secondary address of the laboratory performing this analysis, if applicable. This would include additional address information (e.g., suite, maildrop, etc.).

Applicable Node(s):

ContactInformation

DATA ELEMENT	DESCRIPTION
LabAnalysisID	
Format: Identifier	
Type: Required	
Definition:	A laboratory-defined identifier for an analysis that uniquely identifies a single run for a single sample aliquot or standard. This identifier must be unique for at least all of the analyses reported in a single deliverable, in the context of one method.
Applicable Node(s):	
Analysis	Example: A LIMS-assigned value or a value manually assigned by laboratory personnel. It could reference a run number or a page number from a laboratory notebook.
ReportedResult	If there is any ambiguity about which analysis underlies this result, the LabAnalysisID of this analysis. Example: To identify from which of several dilutions the reported result is chosen.
LabAnalyteID	
Format: Identifier	
Type: Required for Traceability	
Definition:	A laboratory-defined identifier for the analyte.
Applicable Node(s):	
ReportedResult	This identifier gives traceability into the laboratory's systems.
Analyte	
AnalyteGroup	
PeakComparison	LabAnalyteID for the analyte to compare to. If not specified, it is assumed to be the same as the analyte for Peak this PeakComparison is in.
AnalyteComparison	LabAnalyteID for the analyte to compare to.

DATA ELEMENT	DESCRIPTION

LabCity

Format: Text

Type:

Definition: The city in which the laboratory performing the analysis is located.

Applicable Node(s):

ContactInformation

LabContract

Format: Text

Type:

Definition: A client-defined contract number that specifies the contract or agreement under which the laboratory analyzes the samples.

Applicable Node(s):

Header A client-defined contract number under which the data in this data package is reported to the client.

SamplePlusMethod Same as Header, except applied on a per sample basis.

LabContractModificationDescription

Format: Text

Type:

Definition: Text that describes any modifications made to the laboratory's contract.

Applicable Node(s):

Header

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

LabContractModificationID

Format: Text

Type:

Definition: A client-defined identifier that identifies modifications made to the laboratory's contract.

Applicable Node(s):

Header

SamplePlusMethod

LabCountry

Format: Text

Type:

Definition: The country in which the laboratory performing the analysis is located.

Applicable Node(s):

ContactInformation

LabDataPackageID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for this data deliverable package. This identifier applies to a single deliverable.

Applicable Node(s):

Header For example, a document number the laboratory assigns to the physical data package or a file name for an electronic deliverable. Use LabReportingBatch for the logical notion of a group of samples reported as a unit.

LabDataPackageName

Format: Text

Type:

Definition: A laboratory-defined title for this data deliverable package.

Applicable Node(s):

Header

DATA ELEMENT	DESCRIPTION

LabDataPackageVersion

Format: Text

Type:

Definition: If the laboratory resubmits a data package, this data element distinguishes between the different versions.

Applicable Node(s):

Header

LabFileID

Format: Identifier

Type:

Definition: The file, and path if required, name where the raw data from the analysis is stored in the laboratory.

Applicable Node(s):

Analysis

LabID

Format: Identifier

Type: Required

Definition: A client-defined identifier for the laboratory performing and/or reporting this analysis.

Applicable Node(s):

Header This is generally the laboratory that has done all of the work or, if part of the work is subcontracted, the laboratory responsible for the reporting of the data. To be fully reliable, LabIDs must be unique across all potential laboratories.

SamplePlusMethod Same as Header but applied on a per sample basis.

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

ContactInformation

DATA ELEMENT	DESCRIPTION

LabInstrumentQCID

Format: Identifier

Type: Required Conditionally

Definition: A laboratory-defined identifier that uniquely identifies a single instrument Quality Control (QC) analysis or group of analyses.

Applicable Node(s):

InstrumentQC Example: A single instrument QC analysis could include an Instrument_Performance_Check, Continuing_Calibration_Verification, etc. A group of analyses could include an Initial_Calibration.

LabMethodID

Format: Identifier

Type: Required for Traceability

Definition: A laboratory-defined unique identifier for the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

LabMethodName

Format: Text

Type:

Definition: The laboratory-defined descriptive name for the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

LabName

Format: Text

Type:

Definition: The name of the laboratory performing this analysis.

Applicable Node(s):

- **Header**
- **SamplePlusMethod**
- **InstrumentQC**
- **Handling**
- **PreparationPlusCleanup**
- **Analysis**
- **ContactInformation**

LabNarrative

Format: Text

Type:

Definition: A laboratory textual account that describes any appropriate information about anomalies that may have occurred during the analysis or review of the data in the electronic data deliverable.

Applicable Node(s):

- **Header**

LabPointOfContact

Format: Text

Type:

Definition: The person at the laboratory who takes final responsibility for the data.

Applicable Node(s):

- **ContactInformation**

DATA ELEMENT	DESCRIPTION

LabPointOfContactElectronicAddress

Format: Text

Type:

Definition: The electronic address (e-mail) of the person at the laboratory who takes final responsibility for the data.

Applicable Node(s):

ContactInformation

LabPointOfContactTitle

Format: Text

Type:

Definition: The job title of the person at the laboratory who takes final responsibility for the data.

Applicable Node(s):

ContactInformation

LabPointOfContactType

Format: LimitedList

Type:

Definition: The type of the person at the laboratory who takes final responsibility for the data.

Applicable Node(s):

ContactInformation Is this the ‘Primary’ PointOfContact or a ’Secondary’ PointOfContact?

DATA ELEMENT	DESCRIPTION

LabQualifiers

Format: Text

Type:

Definition: A laboratory-assigned string of result qualifiers (usually a single character for each qualifier), based on client-defined rules and values.

Applicable Node(s):

ReportedResult

Analyte

AnalyteGroup

Peak

AnalyteComparison

PeakComparison

LabQualifiersDefinition

Format: Text

Type:

Definition: A formal statement of the meaning or significance of any lab qualifier(s) reported by the laboratory.

Applicable Node(s):

Header The following format should be used:
Qualifier:Definition
When reporting more than one definition, each definition should be separated by a semicolon.

LabReceiptDate

Format: Date

Type:

Definition: The date (and time, if required) that the sample was received in the laboratory.

Applicable Node(s):

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

LabReportedDate

Format: Date

Type:

Definition: The date (and time, if required) that the data package was reported by the laboratory to the client.

Applicable Node(s):

Header

LabReportingBatch

Format: Identifier

Type:

Definition: A laboratory-defined identifier that is used to link multiple samples reported as a group by the laboratory. In addition, this batch can be used to link certain quality control (QC) samples to field samples.

Applicable Node(s):

SamplePlusMethod

LabResultStatus

Format: Limited List

Type:

Definition: A laboratory-assigned state or condition for the results of a particular sample and method.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Preliminary’, ‘Final.’

ReportedResult

DATA ELEMENT	DESCRIPTION

LabSampleID

Format: Identifier

Type: Required for Traceability

Definition: A laboratory-defined identifier that uniquely identifies a single sample that is subjected to an analysis.

Applicable Node(s):

SamplePlusMethod The identifier is the primary link into the laboratory's record keeping system. It is not necessarily one-to-one with the ClientSampleID.

LabState

Format: Text

Type:

Definition: The state in which the laboratory performing the analysis is located.

Applicable Node(s):

ContactInformation

LabTelephoneNumber

Format: Text

Type:

Definition: The 10-digit telephone number of the laboratory performing the analysis.

Applicable Node(s):

ContactInformation

LabType

Format: Limited List

Type:

Definition: Text that describes the laboratory analyzing the sample.

Applicable Node(s):

SamplePlusMethod Example Valid Values: 'Field', 'Fixed', 'Mobile.'

ContactInformation

DATA ELEMENT	DESCRIPTION

LabZipCode

Format: Text

Type:

Definition: The ZIP or postal code of the laboratory performing the analysis.

Applicable Node(s):

ContactInformation

LocationID

Format: Identifier

Type:

Definition: A client-defined identifier of the sampling location at a particular site.

Applicable Node(s):

SamplePlusMethod Examples: Operable_Unit, Well, Tank, Station, Facility (building), Installation, Aggregate_Area.

LocationName

Format: Text

Type:

Definition: A client-defined name of the sampling location at a particular site.

Applicable Node(s):

SamplePlusMethod Examples: Operable_Unit, Well, Tank, Station, Facility (building), Installation, Aggregate_Area.

LotNumber

Format: Text

Type:

Definition: A manufacturer-assigned batch number for an analyte or other materials used in a particular analysis.

Applicable Node(s):

Analyte Example: The vendor/manufacturer-assigned lot number for a purchased standard.

PreparationPlusCleanup Example: Florisil cartridge lot number.

DATA ELEMENT	DESCRIPTION

ManualIntegration

Format: Limited List

Type:

Definition: Indicates whether or not manual integration was used.

Applicable Node(s):

- **Analyte** Example Valid Values: ‘Yes’, ‘No.’
- **Peak**

Mass

Format: Numeric

Type:

Definition: The measured mass of this analyte or peak.

Applicable Node(s):

- **Analyte**
- **Peak**
- **PeakComparison**
- **PeakReplicate**

MassChargeRatio

Format: Numeric

Type:

Definition: The mass/charge relationship recorded in Mass Spectrometry (MS) detection.

Applicable Node(s):

- **Peak**
- **PeakComparison**

DATA ELEMENT	DESCRIPTION

MassLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the Mass.

Applicable Node(s):

Analyte

Peak

PeakComparison

PeakReplicate

MassLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the Mass.

Applicable Node(s):

Analyte

Peak

PeakComparison

PeakReplicate

MassLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the Mass limits. Values reported within these limits indicate if the stated or expected data quality objectives for Mass were achieved.

Applicable Node(s):

Analyte

Peak

PeakComparison

PeakReplicate

DATA ELEMENT	DESCRIPTION

MassUnits

Format: Limited List

Type:

Definition: Units for Mass.

Applicable Node(s):

- **Analyte**
- **Peak**
- **PeakComparison**
- **PeakReplicate**

MatrixID

Format: Limited List

Type: Required

Definition: An identifier that provides a more specific description of the sample matrix or media.

Applicable Node(s):

SamplePlusMethod	For example, the general MatrixMedium ‘Aqueous’ could be further broken down and given the MatrixID ‘Water’, ‘Surface_Water’, ‘Ground_Water’, or ‘Drinking_Water.’
Handling	MatrixID of the sample after the handling described by this node.
PreparationPlusCleanup	MatrixID of the aliquot after the preparation or cleanup described by this node.

MatrixMedium

Format: Limited List

Type: Required for Portability

Definition: An identifier of the general sample substrate or media.

Applicable Node(s):

SamplePlusMethod	Example Valid Values:‘Aqueous’, ‘Solid’, ‘Air’, ‘Non_Aqueous’, ‘Biological_Tissue.’
Handling	MatrixMedium of the sample after the handling described by this node.
PreparationPlusCleanup	MatrixMedium of the aliquot after the preparation or cleanup described by this node.

DATA ELEMENT	DESCRIPTION

MeanCalibrationFactor

Format: Numeric

Type:

Definition: The average or mean ratio of the detector response to the amount (mass or concentration) of an analyte.

Applicable Node(s):

Analyte The mean calibration factor for this analyte.

Peak Same as in Analyte, except applied per peak.

MeanCalibrationFactorUnits

Format: Text

Type:

Definition: Units for MeanCalibrationFactor.

Applicable Node(s):

Analyte

Peak

MeanRelativeResponse

Format: Numeric

Type:

Definition: The ratio of the average or mean response of one analyte to another.

Applicable Node(s):

Analyte The mean relative response for this analyte.

MeanRelativeResponseLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the MeanRelativeResponse.

Applicable Node(s):

Analyte

DATA ELEMENT	DESCRIPTION

MeanRelativeResponseLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the MeanRelativeResponse.

Applicable Node(s):

Analyte

MeanRelativeResponseLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the MeanRelativeResponse limits. Values reported within these limits indicate if the stated or expected data quality objectives for MeanRelativeResponse were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

MeanRetentionTime

Format: Numeric

Type:

Definition: The average or mean time between injection and detection for an analyte using chromatography or other techniques.

Applicable Node(s):

Analyte The mean retention time for this analyte.

Peak Same as in Analyte, except applied per peak.

DATA ELEMENT	DESCRIPTION

MeanRetentionTimeLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the MeanRetentionTime.

Applicable Node(s):

Analyte

Peak

MeanRetentionTimeLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the MeanRetentionTime.

Applicable Node(s):

Analyte

Peak

MeanRetentionTimeLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the MeanRetentionTime limits. Values reported within these limits indicate if the stated or expected data quality objectives for MeanRetentionTime were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

DATA ELEMENT	DESCRIPTION

MeanRetentionTimeUnits

Format: Limited List

Type:

Definition: Units for MeanRetentionTime

Applicable Node(s):

Analyte

Peak

MeanRRF

Format: Numeric

Type:

Definition: The average or mean RelativeResponseFactor.

Applicable Node(s):

Analyte The mean RelativeResponseFactor of the analyte.

Peak Same as in Analyte, except applied per peak.

PeakComparison

MeanRRFLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the MeanRRF.

Applicable Node(s):

Analyte

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION
MeanRRFLimitType	
Format: Limited List	
Type:	
Definition:	The organization or entity that is the origin of the MeanRRF limits. Values reported within these limits indicate if the stated or expected data quality objectives for MeanRRF were achieved.
Applicable Node(s):	
Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	
PeakComparison	
MethodBatch	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier that is used to link multiple samples analyzed by one method and treated as a group for quality control (QC) purposes. A method batch should group samples with similar matrices and potential interferences.
Applicable Node(s):	
SamplePlusMethod	This is a broader grouping than a preparation batch. In particular, a reanalysis of a sample stays in the same method batch, while it is likely to be in a different preparation batch. Operationally, this batch associates sample dependent QC such as duplicates and matrix spikes with a group of samples that may or may not be prepared at the same time.

DATA ELEMENT	DESCRIPTION

MethodCategory

Format: Limited List

Type:

Definition: The general class or common name for the group of analytes being measured by a given method for the sample.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘VOAs’, ‘SVOAs’, ‘Metals’, ‘PCBs’, ‘PESTs.’

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

MethodCode

Format: Limited List

Type:

Definition: The published reference code of the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

MethodID

Format: Limited List

Type: Required for Portability

Definition:	The published, unique identifier (usually consisting of numbers or a combination of letters and numbers) for the method used by the laboratory to analyze the sample.
Applicable Node(s):	
SamplePlusMethod	Example Valid Value: '8260B.' If no published reference method identification number is available then the ClientMethodID data element must be used.
InstrumentQC	
Handling	
PreparationPlusCleanup	
Analysis	

MethodLevel

Format: Limited List

Type:

Definition:	The approximate level of analytes in the sample, usually specified in client-defined concentration ranges and determined via a screening procedure.
Applicable Node(s):	
SamplePlusMethod	Example Valid Values: 'Low', 'Medium', 'High.'

DATA ELEMENT	DESCRIPTION

MethodModificationDescription

Format: Text

Type:

Definition: Text that identifies any modifications made to the published reference method.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

MethodModificationID

Format: Text

Type:

Definition: A client-defined identifier that identifies modifications made to the published reference method.

Applicable Node(s):

SamplePlusMethod

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

MethodName

Format: Limited List

Type:

Definition: The published name or title of the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod Example Valid Value: 'Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS).' If no published reference method name is available then the ClientMethodName data element should be used.

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

MethodSource

Format: Limited List

Type: Required for Portability

Definition: The author or publishing agency of the method used by the laboratory to analyze the sample.

Applicable Node(s):

SamplePlusMethod Example Valid Value: 'USEPA_OSW.' If no published reference method source is available then the ClientMethodSource data element must be used.

InstrumentQC

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

MethodType

Format: Limited List

Type:

Definition: A term that identifies the technology or method classification of the method used by the laboratory to analyze the sample.

Applicable Node(s):

- **SamplePlusMethod** — Example Valid Values: ‘GC/MS’, ‘GC/MS_SIM’, ‘ICP/AES’, ‘ICP/MS’, ‘IR.’
- **InstrumentQC**
- **Handling**
- **PreparationPlusCleanup**
- **Analysis**

MethodVersion

Format: Limited List

Type: Required for Portability

Definition: The version or revision of the method used by the laboratory to analyze the sample.

Applicable Node(s):

- **SamplePlusMethod**
- **InstrumentQC**
- **Handling**
- **PreparationPlusCleanup**
- **Analysis**

MobilePhase

Format: Text

Type:

Definition: The mobile phase composition used for High Performance Liquid Chromatography (HPLC), or other similar procedures.

Applicable Node(s):

- **Analysis**

DATA ELEMENT	DESCRIPTION

NumberDilutions

Format: Numeric

Type:

Definition: The number of dilutions done to the sample aliquot.

Applicable Node(s):

Analysis

OrganismLength

Format: Numeric

Type:

Definition: The length of an organism.

Applicable Node(s):

SamplePlusMethod

OrganismLengthUnits

Format: Limited List

Type:

Definition: Units for OrganismLength.

Applicable Node(s):

SamplePlusMethod

OrganismPortion

Format: Limited List

Type:

Definition: The portion of an organism used for analysis.

Applicable Node(s):

SamplePlusMethod

DATA ELEMENT	DESCRIPTION
OrganismSex	
Format: Limited List	
Type:	
Definition:	The sex of an organism used in the analysis.
Applicable Node(s):	
SamplePlusMethod	Example Valid Values: ‘Male’ or ‘Female.’
OriginalClientSampleID	
Format: Identifier	
Type: Required Conditionally	
Definition:	The client-defined identifier of the original regular sample from which the Quality Control (QC) sample was derived.
Applicable Node(s):	
SamplePlusMethod	For a method QC sample of QCCategory Duplicate, Serial_Dilution, Spike, or Spike_Duplicate, there would normally be an associated regular sample the QC sample is derived from. This sample is called the original. The value of OriginalClientSampleID matches that of the ClientSampleID for this original sample.
OriginalLabAnalysisID	
Format: Identifier	
Type: Required Conditionally	
Definition:	The laboratory analysis identifier (LabAnalysisID) of a previous or original analysis this analysis is based on.
Applicable Node(s):	
Analysis	This data element would only be used for AnalysisType equal to ‘Dilution-##’ or ‘Reinjection-##’, where ## can be any integer starting at ‘01' and incrementing up to ‘99.’

DATA ELEMENT	DESCRIPTION

OriginalLabSampleID

Format: Identifier

Type: Required Conditionally

Definition: The laboratory-defined identifier of the original sample from which the Quality Control (QC) sample was derived.

Applicable Node(s):

SamplePlusMethod For a method QC sample with QCCategory Duplicate, Serial_Dilution, Spike or Spike_Duplicate there would normally be an associated regular sample the QC sample is derived from. This sample is called the original. The value of OriginalLabSampleID matches that of the LabSampleID for this original sample. For a method QC sample with QCCategory Blank_Spike_Duplicate, the value of OriginalLabSampleID matches that of the LabSampleID for the associated Blank_Spike.

Peak

Format:

Type:

Definition: A parent data element that identifies and reports the actual measurement data related to the analysis of analyte peaks.

Applicable Node(s):

Analyte

PeakComparison

Format:

Type:

Definition: A parent data element that identifies cross-peak comparisons (e.g., abundance ratios, inter-peak resolutions).

Applicable Node(s):

Peak

DATA ELEMENT	DESCRIPTION
PeakID	
Format: Identifier	
Type: Required Conditionally	
Definition:	A laboratory-defined identifier that identifies a peak associated with an analyte. Its value should be unique among all peaks for one analyte within a run sequence, but not necessarily have physical meaning.
Applicable Node(s):	
Peak	Examples: Nominal mass for GCMS peaks, integer wavelength for ICP peaks, sequence number (1, 2, ...) for multicomponent GC peaks. PeakID is conceptually similar to ClientAnalyteID, except it identifies a peak rather than an analyte.
ReportedResult	If there is any ambiguity about which peak underlies this result, the PeakID of that peak.
Analyte	If there is any ambiguity about which peak underlies this analyte's result, the PeakID of that peak.
PeakComparison	Peak identifier for the peak to compare to. It is combined with the LabAnalyteID (or ClientAnalyteID) in the same PeakComparison node to fully specify the peak to compare to.
PeakRatio	
Format: Numeric	
Type:	
Definition:	The ratio of the response of two peaks.
Applicable Node(s):	
Peak	
PeakComparison	The response of the peak this PeakComparison node is in as a ratio of the response of the peak identified by the PeakID and LabAnalyteID (or ClientAnalyteID) in this node.

DATA ELEMENT	DESCRIPTION

PeakRatioLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the PeakRatio.

Applicable Node(s):

Peak

PeakComparison

PeakRatioLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the PeakRatio.

Applicable Node(s):

Peak

PeakComparison

PeakRatioLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PeakRatio limits. Values reported within these limits indicate if the stated or expected data quality objectives for PeakRatio were achieved.

Applicable Node(s):

Peak Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

PeakComparison

PeakReplicate

Format:

Type:

Definition: A parent data element related to multiple peak measurements (e.g., multiple exposure readings).

Applicable Node(s):

Peak

DATA ELEMENT	DESCRIPTION

PeakReplicateID

Format: Identifier

Type: Required Conditionally

Definition: A laboratory-defined identifier that identifies a single peak measurement from a series of replicate measurements.

Applicable Node(s):

PeakReplicateID

PercentBreakdown

Format: Numeric

Type:

Definition: The percent breakdown or decomposition of an analyte.

Applicable Node(s):

Analyte	Example: DDT breakdown as reported for pesticide methods.
Peak	The percent breakdown of an analyte when results are measured per peak.

PercentBreakdownLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the PercentBreakdown.

Applicable Node(s):

Analyte

Peak

DATA ELEMENT	DESCRIPTION

PercentBreakdownLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentBreakdown limits. Values reported within these limits indicate if the stated or expected data quality objectives for PercentBreakdown were achieved.

Applicable Node(s):

Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	

PercentDifference

Format: Numeric

Type:

Definition: The difference between two measured values as a percentage of one of them. The denominator value is usually the more certain one, although details can be method specific.

Applicable Node(s):

ReportedResult	
Analyte	Can be applied to the results of analyses in an analysis group rather than a QC sample and original pair.
Peak	Can be used when results are measured per peak.
PeakComparison	Can be used to compare values in two PeakComparison elements.

PercentDifferenceLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the PercentDifference.

Applicable Node(s):

ReportedResult

Analyte

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION

PercentDifferenceLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the PercentDifference.

Applicable Node(s):

ReportedResult

Analyte

Peak

PeakComparison

PercentDifferenceLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentDifference limits. Values reported within these limits indicate if the stated or expected data quality objectives for PercentDifference were achieved.

Applicable Node(s):

ReportedResult Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Analyte

Peak

PeakComparison

PercentMatch

Format: Numeric

Type:

Definition: The percent match of an analyte as compared with a library mass spectrum.

Applicable Node(s):

Analyte

DATA ELEMENT	DESCRIPTION
PercentRatio	
Format: Numeric	
Type:	
Definition:	The ratio of the response of two peaks, expressed as a percentage.
Applicable Node(s):	
Peak	
PeakComparison	The response of the peak this PeakComparison node is in as a percentage of the response of the peak identified by the PeakID and ClientAnalyteID in this node. Example: Used with mass spectral peaks in System Monitoring Compounds.
PercentRatioLimitHigh	
Format: Numeric	
Type:	
Definition:	The uppermost boundary or limit used for the PercentRatio.
Applicable Node(s):	
Peak	
PeakComparison	
PercentRatioLimitLow	
Format: Numeric	
Type:	
Definition:	The lowest boundary or limit used for the PercentRatio.
Applicable Node(s):	
Peak	
PeakComparison	

DATA ELEMENT	DESCRIPTION

PercentRatioLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentRatio limits. Values reported within these limits indicate if the stated or expected data quality objectives for PercentRatio were achieved.

Applicable Node(s):

Peak Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

PeakComparison

PercentRecovery

Format: Numeric

Type:

Definition: The recovery of an analyte expressed as a percentage of the amount added. If a numeric result cannot be calculated then the PercentRecoveryType data element should be used.

Applicable Node(s):

ReportedResult For method QC of QCCategory Blank_Spike and Blank_Spike_Duplicate, the result as a percentage of the amount added. For method QC of QCCategory Spike and Spike_Duplicate, the spiked result minus the original result as a percentage of the ExpectedResult.

Analyte Same as in ReportedResult except applied to the results from an analysis such as a surrogate or analyses in an analysis group rather than a QC sample and original pair.

Peak Same as in Analyte when results are measured per peak.

DATA ELEMENT	DESCRIPTION

PercentRecoveryLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the PercentRecovery..

Applicable Node(s):

ReportedResult

Analyte

Peak

PercentRecoveryLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the PercentRecovery.

Applicable Node(s):

ReportedResult

Analyte

Peak

PercentRecoveryLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentRecovery limits. Values reported within these limits indicate if the stated or expected data quality objectives for PercentRecovery were achieved.

Applicable Node(s):

ReportedResult Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Analyte

Peak

DATA ELEMENT	DESCRIPTION

PercentRecoveryType

Format: Limited List

Type:

Definition: Would be used to report non-numeric PercentRecovery results when the Percent Recovery was calculated but a numerical value could not be determined.

Applicable Node(s):

ReportedResult	Example Valid Value: 'Not_Calculable.'
Analyte	
Peak	

PercentRSD

Format: Numeric

Type:

Definition: The standard deviation of a set of values divided by their mean, expressed as a percentage.

Applicable Node(s):

Analyte	Used for an analyte in AnalysisGroup.
Peak	Used for an analyte, except applied per peak.
PeakComparison	Same as in Peak except applied to PeakComparison values.

PercentRSDLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the PercentRSD.

Applicable Node(s):

Analyte

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION

PercentRSDLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the PercentRSD.

Applicable Node(s):

Analyte

Peak

PeakComparison

PercentRSDLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentRSD limits. Values reported within these limits indicate if the stated or expected objectives for PercentRSD were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

PeakComparison

PercentValley

Format: Numeric

Type:

Definition: The resolution between this analyte and another one, as a percentage of the shorter one. The second analyte is assumed to be known based on the method.

Applicable Node(s):

Analyte

Peak

PeakComparison The resolution or valley between the peak this PeakComparison node is in and the peak identified by the PeakID and LabAnalyteID in this node as a percentage of the height of the shorter one.

DATA ELEMENT	DESCRIPTION

PercentValleyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit for the PercentValley.

Applicable Node(s):

Analyte

Peak

PeakComparison

PercentValleyLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the PercentValley limits. Values reported within these limits indicate if the stated or expected data quality objectives for PercentValley were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

PeakComparison

PhaseAnalyzed

Format: Limited List

Type:

Definition: That portion or fraction of a multiphase sample that was actually analyzed.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Upper’, ‘Middle’, ‘Lower.’

DATA ELEMENT	DESCRIPTION

PreparationBatch

Format: Identifier

Type:

Definition: A laboratory-defined identifier that is used to link multiple sample aliquots that are prepared together for analysis by one method. "Together" implies similarity of time, place, and manner of preparation.

Applicable Node(s):

Analysis

PreparationPlusCleanup

PreparationID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for this preparation event for this sample aliquot.

Applicable Node(s):

PreparationPlusCleanup

PreparationPlusCleanup

Format:

Type:

Definition: A parent data element that describes a preparation or cleanup process as part of an analysis.

Applicable Node(s):

Analysis

PreparationPlusCleanupType

Format: Limited List

Type:

Definition: Whether or not the data in this node is related to a preparation or cleanup activity.

Applicable Node(s):

PreparationPlusCleanup Example Valid Values: 'Preparation', 'Cleanup.'

DATA ELEMENT	DESCRIPTION

PreparationType

Format: Text

Type:

Definition: A client-defined description used to define the specific preparation performed when multiple options are given within the referenced method.

Applicable Node(s):

Analysis	This description is used to specify which preparation method was used when such preparation method details are part of the analysis (instrumental) method. When client preparation methods are available, this description is used to identify what method options were used within the preparation method.
PreparationPlusCleanup	

PreparationUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the Result, by which the Result may differ from the true value due to all effects, other than the instrumental analysis, related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult	Expressed as an offset to the Result (y) in the form: Result ± positive numeric value ($y \pm a$).
Analyte	Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

DATA ELEMENT	DESCRIPTION

PreparationUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, at which the PreparationUncertainty was determined.

Applicable Node(s):

ReportedResult	Reported as a value between 0 and 100%.
Analyte	
Peak	
PeakReplicate	

PreparationUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported PreparationUncertainty.

Applicable Node(s):

ReportedResult	This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality) should also be included; statistical experimental design (e.g., number of replicate measurements).
Analyte	
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION

PreparationUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the Result.

Applicable Node(s):

ReportedResult Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the Result, ‘Other_Interval’ when the interval is not centered on the Result.

Analyte

Peak

PeakReplicate

PreparationUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the Result may differ from the true value due to all effects, other than the instrumental analysis, related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult Expressed as a upper limit to the Result in the form: Result (y) < Upper Result limit (a_H). When both Upper and Lower Result limits are reported, the result should appear as: Lower Limit Result (a_L) < Result (y) < Upper Limit Result (a_H).

Analyte Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.

Peak Same as in Analyte when results are measured per peak.

PeakReplicate

DATA ELEMENT	DESCRIPTION

PreparationUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the Result may differ from the true value due to all effects, other than the instrumental analysis, related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult	Expressed as a lower limit to the Result in the form: Lower Result limit (a_L) < Result (y). When both Upper and Lower Result limits are reported, the result should appear as: Lower Limit Result (a_L) < Result (y) < Upper Limit Result (a_H).
Analyte	Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

PreparationUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the PreparationUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

ReportedResult	Example Valid Values: ‘Category A’ where the estimate of the PreparationUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the PreparationUncertainty is determined using some other method (in whole or in part).
Analyte	
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION

PreparationUncertaintyUnits

Format: Limited List

Type:

Definition: Units for PreparationUncertainty.

Applicable Node(s):

ReportedResult	If the client specifies that the PreparationUncertaintyUnits must be the same as the ResultUnits, the PreparationUncertaintyUnits need not be specified.
Analyte	Same as in ReportedResult.
Peak	Same as in ReportedResult.
PeakReplicate	

PreparedDate

Format: Date

Type:

Definition: The date (and time, if required) of the preparation of this sample aliquot. Preparation is used generally to include method specific techniques such as extraction, digestion, and separation. If prepared over a range of dates, this is the start date.

Applicable Node(s):

Analysis

PreparationPlusCleanup

PreparedEndDate

Format: Date

Type:

Definition: The date (and times, if required) of the end of the preparation period for the sample aliquot, if the sample was prepared over a period of time.

Applicable Node(s):

Analysis

PreparationPlusCleanup

DATA ELEMENT	DESCRIPTION

Preservative

Format: Text

Type:

Definition: The chemical compound that was added to the sample to protect against decay or decomposition.

Applicable Node(s):

SamplePlusMethod

PreservedBy

Format: Text

Type:

Definition: The organization that added preservative to the sample.

Applicable Node(s):

SamplePlusMethod

PriorityID

Format: Limited List

Type:

Definition: A client-defined term that identifies the priority assigned to this data. The priority may affect the desired turn around time and the cost of the analysis.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Rush’, ‘Normal.’

ProcedureID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for the laboratory’s Standard Operating Procedure (SOP) for this method of analysis.

Applicable Node(s):

Analysis

Handling

PreparationPlusCleanup

DATA ELEMENT	DESCRIPTION

ProcedureName

Format: Text

Type:

Definition: A descriptive title of the laboratory's Standard Operating Procedure (SOP) for the method used for analysis.

Applicable Node(s):

Analysis

Handling

PreparationPlusCleanup

ProjectID

Format: Identifier

Type:

Definition: A client-defined identifier for a project reporting a particular set of data. Typically, a project consists of samples from one site collected over some defined period of time.

Applicable Node(s):

Header The project identifier for the samples being reported in this deliverable.

SamplePlusMethod Same as Header, except on a per sample basis.

ProjectName

Format: Text

Type:

Definition: A descriptive name or label for the project for which data is being reported for.

Applicable Node(s):

Header

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

QCCategory

Format: Limited List

Type: Required for Portability

Definition: A term that identifies the basic properties or category of a particular method Quality Control (QC) sample.

Applicable Node(s):

SamplePlusMethod

Example Valid Values:

1. ‘Blank’ - A QC sample with ‘nothing’ in it. Examples: Field, equipment, method (reagent), sulfur and storage blanks.
2. ‘Blank_Spike’ - A QC sample with a known amount added to a Blank. Examples: laboratory control samples, QC check samples, and interference check samples.
3. ‘Duplicate’ - A reanalysis of a regular sample done for QC purposes. Examples: duplicates and splits.
4. ‘Blank_Spike_Duplicate’ - A reanalysis of a BlankSpike.
5. ‘Serial_Dilution’ - A dilution and reanalysis of a regular sample done for QC purposes.
6. ‘Spike’ - A reanalysis of a regular sample with a known amount added and done for QC purposes. Examples: matrix spikes, post digestion spikes, and analytical spikes.
7. ‘Spike_Duplicate’ - A second reanalysis of a regular sample with a known amount added and done for QC purposes. There must be another sample with QCCategory ‘Spike’ with the same original sample.

DATA ELEMENT	DESCRIPTION

QCLinkage

Format: Limited List

Type: Required for Portability

Definition:	For a Quality Control (QC) sample, specifies which batch is the basis for the association between the QC sample and the regular samples.
Applicable Node(s):	
SamplePlusMethod	Allowed Valid Values include the following data elements that define batches: ‘SamplingBatch’, ‘EquipmentBatch’, ‘ShippingBatch’, ‘LabReportingBatch’, ‘MethodBatch’, ‘HandlingBatch’, ‘PreparationBatch’, ‘AnalysisBatch’, ‘CleanupBatch’, ‘StorageBatch.’ If QCLinkage is ‘HandlingBatch’, there should be a HandlingType element in the SamplePlusMethod node whose value clarifies which type of handling batch is intended. Example: In SamplePlusMethod, if the QCType is Duplicate, the QCCategory is Duplicate and the QCLinkage is MethodBatch, a reader knows that this data is for a client-defined type of QC called a Duplicate, that it is processed with rules typical for Duplicates and that it is to be associated with other SamplePlusMethod elements with the same value for the MethodBatch field. QCLinkage is most useful if the batch it names is a required element, based on implementation rules. The correct linkage for a field QC sample may not be known to the laboratory, so must be merged with laboratory data at a later time.
InstrumentQC	Same as in SamplePlusMethod except allowed Valid Values for instrument QC are ‘CleanupBatch’, ‘PreparationBatch’, ‘AnalysisBatch’, and ‘RunBatch.’ If QCLinkage is ‘CleanupBatch’, there should be a CleanupType element in InstrumentQC whose value clarifies which type of cleanup batch is intended.

DATA ELEMENT	DESCRIPTION

QCType

Format: Limited List

Type: Required

Definition: The client-defined term that identifies the specific type of sample being analyzed.

Applicable Node(s):

SamplePlusMethod In the context of the ClientMethodID and MatrixID, this term determines all special processing rules for the sample. The default Valid Value is 'Field_Sample' for a regular sample. The presence of any other term in this field defines the sample as a method, client or performance QC sample. A laboratory may not know that certain samples are QC. In this case the laboratory reports them as regular samples ('Field_Sample') and their type is changed later, possibly by the validator.

InstrumentQC For instrument QC, a client-defined term that specifies what type of instrument QC data follows. In the context of the ClientMethodID, the value must imply enough detail for the reader to understand the method specific details of the following AnalysisGroup, Analysis, PrepPlusCleanup, Analyte, Peak, PeakComparison, and AnalyteComparison elements.

QuantitationBasis

Format: Limited List

Type:

Definition: The conditions upon which sample quantitation is performed (e.g., using internal standards).

Applicable Node(s):

Analysis Example valid values: 'Internal_Standard' or 'External_Standard.'

Analyte

DATA ELEMENT	DESCRIPTION
QuantitationLimit	
Format: Numeric	
Type:	
Definition:	The quantitation limit for the analyte being measured. Quantitation limits are defined in terms of a the lowest reported value of the analyte that can be reliably determined within a specified degree of uncertainty.
Applicable Node(s):	
ReportedResult	
Analyte	Within AnalysisGroup, applies to a quantitation limit value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
QuantitationLimitType	
Format: Limited List	
Type:	
Definition:	A term that identifies how the quantitation limit was determined or reported.
Applicable Node(s):	
ReportedResult	Example Valid Values: ‘CRQL’, ‘PQL.’
Analyte	
Peak	
QuantitationLimitUnits	
Format: Limited List	
Type:	
Definition:	Units for QuantitationLimit.
Applicable Node(s):	
ReportedResult	If the client specifies that the QuantitationLimitUnits must be the same as the ResultUnits, the QuantitationLimitUnits need not be specified.
Analyte	Same as in ReportedResult.
Peak	Same as in ReportedResult.

DATA ELEMENT	DESCRIPTION

Quarantine

Format: Limited List

Type:

Definition: Indicates whether or not the sample, as received by the laboratory, is to be quarantined.

Applicable Node(s):

SamplePlusMethod Example Valid Values: ‘Yes’, ‘No.’

Quench

Format: Numeric

Type:

Definition: The result of quench calculation for scintillation counters.

Applicable Node(s):

Analysis

ReferenceDate

Format: Date

Type:

Definition: The date (and time, if required) used for decay correction in radiochemical analyses.

Applicable Node(s):

Analysis

RelativeResponse

Format: Numeric

Type:

Definition: The ratio of the response of one analyte to another.

Applicable Node(s):

Analyte The relative response for this analyte, based on the assumption that the method specifies the analyte to compare to and which peaks to use.

DATA ELEMENT	DESCRIPTION

RelativeResponseLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the RelativeResponse.

Applicable Node(s):

Analyte

RelativeResponseLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the RelativeResponse.

Applicable Node(s):

Analyte

RelativeResponseLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the RelativeResponse limits. Values reported within these limits indicate if the stated or expected data quality objectives for RelativeResponse were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

DATA ELEMENT	DESCRIPTION

RelativeRetentionTime

Format: Numeric

Type:

Definition: The ratio of two retention times. A relative retention time is the ratio of the retention time of a compound to another.

Applicable Node(s):

Analyte	The relative retention time for this analyte, based on the assumption that the method specifies the analyte to compare to and which peaks to use.
Peak	The relative retention time for this peak, based on the assumption that the method specifies the peak to compare to.
PeakComparison	The relative retention time of the peak this PeakComparison node is in compared to the peak identified by the PeakID and LabAnalyteID (or ClientAnalyteID) in this node.

RelativeRetentionTimeLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the RelativeRetentionTime.

Applicable Node(s):

Analyte

Peak

PeakComparison

RelativeRetentionTimeLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the RelativeRetentionTime.

Applicable Node(s):

Analyte

Peak

PeakComparison

DATA ELEMENT	DESCRIPTION

RelativeRetentionTimeLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the RelativeRetentionTime limits. Values reported within these limits indicate if the stated or expected data quality objectives for RelativeRetentionTime were achieved.

Applicable Node(s):

Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	
PeakComparison	

ReportedResult

Format:

Type:

Definition: A parent data element that reports the final reportable results of a method.

Applicable Node(s):

SamplePlusMethod

ReportingLimit

Format: Numeric

Type:

Definition: The reporting limit of the analyte being measured. Reporting limits are defined in terms of a number below which data is typically reported as ‘not detected’ for the analyte being measured.

Applicable Node(s):

ReportedResult	
Analyte	Within AnalysisGroup, applies to a reporting limit value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.

DATA ELEMENT	DESCRIPTION

ReportingLimitType

Format: Limited List

Type:

Definition: A term that identifies how the reporting limit was determined or reported.

Applicable Node(s):

ReportedResult	Example Valid Values: ‘MDL’, ‘PQL.’
Analyte	
Peak	

ReportingLimitUnits

Format: Limited List

Type:

Definition: Units for ReportingLimit.

Applicable Node(s):

ReportedResult	If the client specifies that the ReportingLimitUnits must be the same as the ResultUnits, the ReportingLimitUnits need not be specified.
Analyte	Same as in ReportedResult.
Peak	Same as in ReportedResult.

RequestorID

Format: Identifier

Type:

Definition: An identifier for the organization that requested this sample analysis.

Applicable Node(s):

SamplePlusMethod	May not be the same as the client, who specifies the SOW to follow.

DATA ELEMENT	DESCRIPTION

RequesterName

Format: Text

Type:

Definition: The name for the organization that requested this sample analysis.

Applicable Node(s):

SamplePlusMethod

Resolution

Format: Numeric

Type:

Definition: The resolution is often defined in terms of the instrument's ability to differentiate one analyte from another for a given method and is often dependent on the smallest amount of input signal change that the instrument can reliably detect.

Applicable Node(s):

Analysis	For example, in isotopic alpha spectroscopy, the width of the tracer peak.
Analyte	A possibly sample and method dependent estimate of the resolution of the instrument that applies to the analysis and analyte.
Peak	Resolution for this peak. Details of how resolution is computed depend on the method.
PeakReplicate	

ResolutionLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the Resolution.

Applicable Node(s):

Analysis

Analyte

Peak

PeakReplicate

DATA ELEMENT	DESCRIPTION

ResolutionLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the Resolution.

Applicable Node(s):

Analysis

Analyte

Peak

PeakReplicate

ResolutionLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the Resolution limits. Values reported within these limits indicate if the stated or expected data quality objectives for Resolution were achieved.

Applicable Node(s):

Analysis Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Analyte

Peak

PeakReplicate

ResolutionType

Format: Limited List

Type:

Definition: The basis by which the estimated resolution was determined or reported.

Applicable Node(s):

Analysis

Analyte

Peak Example Valid Values: ‘Peak Width at 10% Peak Height.’

PeakReplicate

DATA ELEMENT	DESCRIPTION

ResolutionUnits

Format: Limited List

Type:

Definition: Units for Resolution.

Applicable Node(s):

- **Analysis**
- **Analyte**
- **Peak**
- **PeakReplicate**

Response

Format: Numeric

Type:

Definition: The response or output from a detector.

Applicable Node(s):

- **Analyte**
- **Peak**
- **PeakComparison**
- **PeakReplicate**

ResponseLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the Response.

Applicable Node(s):

- **Analyte**
- **Peak**
- **PeakComparison**
- **PeakReplicate**

DATA ELEMENT	DESCRIPTION

ResponseLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the Response.

Applicable Node(s):

Analyte

Peak

PeakComparison

PeakReplicate

ResponseLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the Response limits. Values reported within these limits indicate if the stated or expected data quality objectives for Response were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

PeakComparison

PeakReplicate

ResponseType

Format: Limited List

Type:

Definition: A term that identifies if the response has been adjusted or corrected (i.e., for background).

Applicable Node(s):

Analyte Example Valid Values: ‘Corrected.’

Peak

PeakComparison

PeakReplicate

DATA ELEMENT	DESCRIPTION

ResponseUnits

Format: Limited List

Type:

Definition: Units for Response.

Applicable Node(s):

- **Analyte**
- **Peak**
- **PeakComparison**
- **PeakReplicate**

Result

Format: Numeric

Type:

Definition: The final calculated result for an analyte accounting for all sample aliquot amounts, dilutions, moisture determinations, etc.

Applicable Node(s):

ReportedResult	The final calculated result for an analyte for a method accounting for all sample aliquot amounts, dilutions, moisture determinations, etc.
Analyte	Same as in ReportedResult when results are calculated based on a single analysis. Within AnalysisGroup, applies to the mean or other value computed from several analyses.
AnalyteGroup	Same as in ReportedResult when results are reported based on two or more measured analytes.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

DATA ELEMENT	DESCRIPTION
ResultBasis	
Format: Limited List	
Type:	
Definition:	The basis upon which the final results were calculated.
Applicable Node(s):	
Analysis	Example Valid Values: ‘Dry’, ‘Wet’, ‘Total’, ‘Dissolved.’
ReportedResult	
ResultLimitHigh	
Format: Numeric	
Type:	
Definition:	The uppermost boundary or limit used for the result.
Applicable Node(s):	
ReportedResult	
Analyte	
Peak	
PeakReplicate	
ResultLimitLow	
Format: Numeric	
Type:	
Definition:	The lowest boundary or limit for the result.
Applicable Node(s):	
ReportedResult	
Analyte	
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION
ResultLimitType	
Format: Limited List	
Type:	
Definition:	The organization or entity that is the origin of the Result limits. Values reported within these limits indicate if the stated or expected data quality objectives for Result were achieved.
Applicable Node(s):	
ReportedResult	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Analyte	
Peak	
PeakReplicate	
ResultType	
Format: Limited List	
Type: Required	
Definition:	Specifies whether this analyte was detected or not detected. For positive detections, specifies whether the result is equal to, greater than, or less than the value reported. Can also be used to report method non-numeric results.
Applicable Node(s):	
ReportedResult	Example valid values: For detections - ‘=’, ‘>’, ‘<’; for non-detects - ‘Not_Detected’; for non-numeric results - ‘Pass’ or ‘Fail’, ‘Positive’ or ‘Negative’, ‘Present’ or ‘Absent.’
Analyte	
AnalyteGroup	
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION

ResultUncertainty

Format: Numeric

Type:

Definition: The estimated amount, expressed as a symmetric interval centered on the Result, by which the Result may differ from the true value due to all effects related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult	Expressed as an offset to the Result (*y*) in the form: Result ± positive numeric value ($y \pm a$).
Analyte	Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

ResultUncertaintyConfidenceLevel

Format: Numeric

Type:

Definition: The confidence level, reported as a percentage, at which the ResultUncertainty was determined.

Applicable Node(s):

ReportedResult	Reported as a value between 0 and 100%.
Analyte	
Peak	
PeakReplicate	

DATA ELEMENT	DESCRIPTION

ResultUncertaintyDetermination

Format: Text

Type:

Definition: Describes the method used by the laboratory to determine the reported ResultUncertainty.

Applicable Node(s):

ReportedResult This should include the following: any equations that were used defining all symbols used; any assumptions required for the equation (e.g., normality) should also be included; statistical experimental design (e.g., number of replicate measurements).

Analyte

Peak

PeakReplicate

ResultUncertaintyIntervalType

Format: Limited List

Type:

Definition: Reports whether or not the uncertainty interval or range reported is centered on the Result.

Applicable Node(s):

ReportedResult Example Valid Values: ‘Symmetric_Interval’ when the interval is centered on the Result, ‘Other_Interval’ when the interval is not centered on the Result.

Analyte

Peak

PeakReplicate

DATA ELEMENT	DESCRIPTION

ResultUncertaintyLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit of the estimated amount by which the Result may differ from the true value due to all effects related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult	Expressed as a upper limit to the Result in the form: Result (y) < Upper Result limit (a_H). When both Upper and Lower Result limits are reported, the result should appear as: Lower Limit Result (a_L) < Result (y) < Upper Limit Result (a_H).
Analyte	Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

ResultUncertaintyLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit of the estimated amount by which the Result may differ from the true value due to all effects related to analysis of the sample aliquot by the laboratory.

Applicable Node(s):

ReportedResult	Expressed as a lower limit to the Result in the form: Lower Result limit (a_L) < Result (y). When both Upper and Lower Result limits are reported, the result should appear as: Lower Limit Result (a_L) < Result (y) < Upper Limit Result (a_H).
Analyte	Extended to anything considered to be the result of any analysis. Within AnalysisGroup, applies to a mean or other value computed from several analyses.
Peak	Same as in Analyte when results are measured per peak.
PeakReplicate	

DATA ELEMENT	DESCRIPTION

ResultUncertaintyType

Format: Limited List

Type:

Definition: Whether or not the reported estimate of the ResultUncertainty is directly determined using a statistically-based method or if is based on another method (in whole or in part).

Applicable Node(s):

ReportedResult	Example Valid Values: ‘Category A’ where the estimate of the ResultUncertainty is directly determined using a statistically-based method, ‘Category B’ where the estimate of the ResultUncertainty is determined using some other method (in whole or in part).
Analyte	
Peak	
PeakReplicate	

ResultUncertaintyUnits

Format: Limited List

Type:

Definition: Units for ResultUncertainty.

Applicable Node(s):

ReportedResult	If the client specifies that the ResultUncertaintyUnits must be the same as the ResultUnits, the ResultUncertaintyUnits need not be specified.
Analyte	Same as in ReportedResult.
Peak	Same as in ReportedResult.
PeakReplicate	

DATA ELEMENT	DESCRIPTION

ResultUnits

Format: Limited List

Type:

Definition: Units for Result.

Applicable Node(s):

ReportedResult

Analyte

AnalyteGroup

Peak

PeakReplicate

RetentionTime

Format: Numeric

Type:

Definition: The time between injection and detection for an analyte using chromatography or other techniques.

Applicable Node(s):

ReportedResult In Results, this is the retention time from the analysis underlying this result.

Analyte Same as in ReportedResult. Used when there is a well defined retention time for the analyte, not just for a peak measurement for the analyte. For example, this applies to GC/MS analyses.

Peak Same as in ReportedResult except for a single peak. Used with techniques like GC where there can be multiple peaks with different retention times for one analyte.

RetentionTimeLimitHigh

Format: Numeric

Type:

Definition: The uppermost boundary or limit used for the RetentionTime.

Applicable Node(s):

Analyte

Peak

DATA ELEMENT	DESCRIPTION

RetentionTimeLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the RetentionTime.

Applicable Node(s):

Analyte

Peak

RetentionTimeLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the RetentionTime limits. Values reported within these limits indicate if the stated or expected data quality objectives for RetentionTime were achieved.

Applicable Node(s):

Analyte Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’

Peak

RetentionTimeUnits

Format: Limited List

Type:

Definition: Units for RetentionTime.

Applicable Node(s):

ReportedResult

Analyte

Peak

DATA ELEMENT	DESCRIPTION
RPD	
Format: Numeric	
Type:	
Definition:	The relative percent difference is the absolute value of the difference of two values over the mean of those values, expressed as a percentage. If a numeric result cannot be calculated then the RPDType data element should be used.
Applicable Node(s):	
ReportedResult	Used with method QC of QCCategory Duplicate, Spike_Duplicate, and Blank_Spike_Duplicate.
Analyte	Same as in ReportedResult except applied to the results of analyses in an analysis group rather than a QC sample and original pair.
Peak	Same as in Analyte when results are measured per peak.
PeakComparison	Same as in ReportedResult except used to compare values in two PeakComparison elements.
RPDLimitHigh	
Format: Numeric	
Type:	
Definition:	The uppermost boundary or limit used for the RPD.
Applicable Node(s):	
Analyte	
ReportedResult	
Peak	
PeakComparison	

DATA ELEMENT	DESCRIPTION
RPDLimitLow	
Format: Numeric	
Type:	
Definition:	The lowest boundary or limit used for the RPD.
Applicable Node(s):	
Analyte	
ReportedResult	
Peak	
PeakComparison	
RPDLimitType	
Format: Limited List	
Type:	
Definition:	The organization or entity that is the origin of the RPD limits. Values reported within these limits indicate if the stated or expected data quality objectives for RPD were achieved.
Applicable Node(s):	
Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
ReportedResult	
Peak	
PeakComparison	
RPDType	
Format: Limited List	
Type:	
Definition:	Would be used to report non-numeric RPD results when the RPD was calculated but a numerical value could not be determined as is possible when one of the two values is not detected.
Applicable Node(s):	
ReportedResult	Example Valid Value: ‘Not_Calculable.’
Analyte	
Peak	

DATA ELEMENT	DESCRIPTION
RRF	
Format: Numeric	
Type:	
Definition:	The relative response factor, which is a ratio of two response factors. A response factor is the ratio of the detector response to an amount (mass or concentration) of analyte.
Applicable Node(s):	
Analyte	The relative response factor for this analyte, based on the assumption that the method specifies the analyte to compare to and which peaks to use.
Peak	The relative response factor for this peak, based on the assumption that the method specifies the peak to compare to.
PeakComparison	The relative response factor of the peak this PeakComparison node is in compared to the peak identified by the PeakID and LabAnalyteID (or ClientAnalyteID) in this node.
RRFLimitHigh	
Format: Numeric	
Type:	
Definition:	The uppermost boundary or limit used for the RRF.
Applicable Node(s):	
Analyte	
Peak	
PeakComparison	
RRFLimitLow	
Format: Numeric	
Type:	
Definition:	The lowest boundary or limit used for the RRF.
Applicable Node(s):	
Analyte	
Peak	
PeakComparison	

DATA ELEMENT	DESCRIPTION
RRFLimitType	
Format: Limited List	
Type:	
Definition:	The organization or entity that is the origin of the RRF limits. Values reported within these limits indicate if the stated or expected data quality objectives for RRF were achieved.
Applicable Node(s):	
Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	
PeakComparison	
RunBatch	
Format: Identifier	
Type:	
Definition:	A laboratory-defined identifier that is used to link multiple analyses performed on one instrument and under the control of one initial calibration.
Applicable Node(s):	
Analysis	Example: A batch of samples analyzed on one instrument under the control of one initial calibration or similar InstrumentQC.

DATA ELEMENT	DESCRIPTION

SampleAmount

Format: Numeric

Type:

Definition: The amount (weight or volume) of material as received by a laboratory or as produced by a handling process that will be aliquotted and processed as a sample for analysis.

Applicable Node(s):

SamplePlusMethod	Weight or volume of sample as received by the laboratory. The SampleAmount would not be directly used in the computation of a final result.
Handling	Weight or volume of sample after the handling described by this node.
PreparationPlusCleanup	Weight or volume of sample in the bottle/container used for this preparation. Normally, a sample aliquot would be withdrawn from the sample container for this preparation process, however, the entire bottle/container contents could be used for this aliquot.
Analysis	Weight or volume of sample in the bottle/container used for this analysis. Normally, a sample aliquot would be withdrawn from the sample container for this analysis process; however, the entire bottle/container contents could be used for this aliquot.

SampleAmountUnits

Format: Limited List

Type:

Definition: Units for SampleAmount.

Applicable Node(s):

SamplePlusMethod

Handling

PreparationPlusCleanup

Analysis

DATA ELEMENT	DESCRIPTION

SamplePlusMethod

Format:

Type:

Definition: A parent data element that describes one sample analyzed under the criteria of one primary method.

Applicable Node(s):

Header

SamplingBatch

Format: Identifier

Type:

Definition: A sampler-defined identifier that is used to link multiple samples collected together. Operationally, this batch associates a field blank with a group of samples.

Applicable Node(s):

SamplePlusMethod This value is currently often not known to the laboratory. It might be merged with laboratory data by a validator.

ScreenValue

Format: Numeric

Type:

Definition: The result from a screening analysis of the sample.

Applicable Node(s):

SamplePlusMethod Example: As in an alpha particle screen.

ScreenValueUnits

Format: Limited List

Type:

Definition: Units for ScreenValue.

Applicable Node(s):

SamplePlusMethod

DATA ELEMENT	DESCRIPTION

ShippingBatch

Format: Identifier

Type:

Definition: A sampler-defined identifier that is used to link multiple samples shipped together, such as in the same crate, cooler, or ice chest. Operationally, this batch associates a trip blank with a group of samples.

Applicable Node(s):

SamplePlusMethod This value, as defined by the shippers, is often not known to the laboratory. It might be merged with laboratory data by a validator.

SignalToNoiseRatio

Format: Numeric

Type:

Definition: The ratio of a signal power to the background noise power corrupting the signal.

Applicable Node(s):

Analyte The method will often define how the analyte and background signals are to be measured.

Peak

SignalToNoiseRatioLimitLow

Format: Numeric

Type:

Definition: The lowest boundary or limit used for the SignalToNoiseRatio.

Applicable Node(s):

Analyte

Peak

DATA ELEMENT	DESCRIPTION

SignalToNoiseRatioLimitType

Format: Limited List

Type:

Definition: The organization or entity that is the origin of the SignalToNoiseRatio limits. Values reported within these limits indicate if the stated or expected data quality objectives for SignalToNoiseRatio were achieved.

Applicable Node(s):

Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	

SiteID

Format: Identifier

Type:

Definition: A client-defined identifier for the broadly defined site for which this data is being reported.

Applicable Node(s):

Header	The site identifier for the samples being reported in this deliverable.
SamplePlusMethod	Same as Header, except on a per sample basis.

SiteName

Format: Text

Type:

Definition: A descriptive name for the broadly defined site for which this data is being reported.

Applicable Node(s):

Header	Example: This could describe a geographical place name, building name, landmark, company name, etc.
SamplePlusMethod	Same as Header, except on a per sample basis.

DATA ELEMENT	DESCRIPTION

Solvent

Format: Text

Type:

Definition: The substance(s), usually a liquid, that was used to dissolve another liquid, gas or solid during the extraction of the sample.

Applicable Node(s):

PreparationPlusCleanup

StandardConcentration

Format: Numeric

Type:

Definition: The actual concentration of the standard used for spiking analytes or for preparing other standards.

Applicable Node(s):

Analyte When spiking an analyte(s) into an aliquot or standard, this represents the actual concentration of the analyte in the spiking solution used. This data element is most commonly used in conjunction with the data element AmountAdded.

StandardConcentrationUnits

Format: Limited List

Type:

Definition: Units for StandardConcentration.

Applicable Node(s):

Analyte

DATA ELEMENT	DESCRIPTION

StandardDeviation

Format: Numeric

Type:

Definition: The level of variation for measurements of one analyte.

Applicable Node(s):

Analyte	The level of variation or standard deviation of several measurements of an analyte.
Peak	Same as in Analyte, except applied per peak.
PeakComparison	

StandardDeviationUnits

Format: Limited List

Type:

Definition: Units for StandardDeviation.

Applicable Node(s):

Analyte	If the client specifies that the StandardDeviationUnits must be the same as the ResultUnits, the StandardDeviationUnits need not be specified.
Peak	Same as in Analyte when results are measured per peak.
PeakComparison	Same as in Analyte except as applied to PeakComparison values.

StandardFinalAmount

Format: Numeric

Type:

Definition: The final amount (weight or volume) of a prepared standard.

Applicable Node(s):

Analyte	This is typically used when preparing a standard that will be used as an initial calibration standard, continuing calibration verification standard or other InstrumentQC standard. The concentration of this standard would be determined by multiplying the AmountAdded by the StandardConcentration and then dividing by the StandardFinalAmount. Often, a larger quantity of this standard is prepared than would typically be consumed during a single analysis.

DATA ELEMENT	DESCRIPTION

StandardFinalAmountUnits

Format: Limited List

Type:

Definition: Units for StandardFinalAmount.

Applicable Node(s):

Analyte

StandardID

Format: Identifier

Type:

Definition: A laboratory-defined identifier for a purchased or laboratory-prepared standard, such as a spiking material or a calibration standard, used in this analysis.

Applicable Node(s):

Analyte

Analysis

StandardSource

Format: Text

Type:

Definition: The origin or manufacturer of a standard used in this analysis.

Applicable Node(s):

Analyte

Analysis

StorageBatch

Format: Identifier

Type:

Definition: A laboratory-defined identifier that is used to link multiple samples that are stored together in a defined period of time (e.g., samples stored in the same refrigerator or freezer).

Applicable Node(s):

SamplePlusMethod Operationally, this batch can associate a VOC refrigerator storage blank with a group of VOC samples.

DATA ELEMENT	DESCRIPTION
TailingFactor	
Format: Numeric	
Type:	
Definition:	The unitless factor describing the amount of tailing observed in a chromatographic or other peak.
Applicable Node(s):	
Analyte	The exact equation or formula used may be method specific. The TailingFactor is normally calculated by dividing the peak tail distance by the peak front distance measured at a given peak height (usually at 10% of the peak height).
Peak	
TailingFactorLimitHigh	
Format: Numeric	
Type:	
Definition:	The uppermost boundary or limit used for the TailingFactor.
Applicable Node(s):	
Analyte	
Peak	
TailingFactorLimitType	
Format: Limited List	
Type:	
Definition:	The organization or entity that is the origin of the TailingFactor limits. Values reported within these limits indicate if the stated or expected data quality objectives for TailingFactor were achieved.
Applicable Node(s):	
Analyte	Example Valid Values: ‘Method’, ‘Client’, ‘Laboratory.’
Peak	

DATA ELEMENT	DESCRIPTION
Temperature	
Format: Numeric	
Type:	
Definition:	The temperature at which method is performed.
Applicable Node(s):	
Analysis	The temperature of the Analysis process.
TemperatureUnits	
Format: Limited List	
Type:	
Definition:	Units for Temperature.
Applicable Node(s):	
Analysis	
Wavelength	
Format: Numeric	
Type:	
Definition:	The wavelength (the distance between corresponding points on two successive waves, generally measured from crest to crest) used for an analytical measurement.
Applicable Node(s):	
Analysis	e.g., for UV/VIS, GFAA, ICP.
Analyte	
Peak	
PeakComparison	

DATA ELEMENT	DESCRIPTION

WavelengthUnits

Format: Limited List

Type:

Definition: Units for Wavelength.

Applicable Node(s):

Analysis

Analyte

Peak

PeakComparison

WeightingFactor

Format: Limited List

Type:

Definition: The factor for an analyte used to define how the regression analysis was applied to an initial calibration curve for a method.

Applicable Node(s):

Analyte The weighting factor for this analyte. Example Valid Values: 'Inverse_Of_Concentration', 'Inverse_Square_Of_Concentration.'

Peak Same as in Analyte, except applied per peak.

Yield

Format: Numeric

Type:

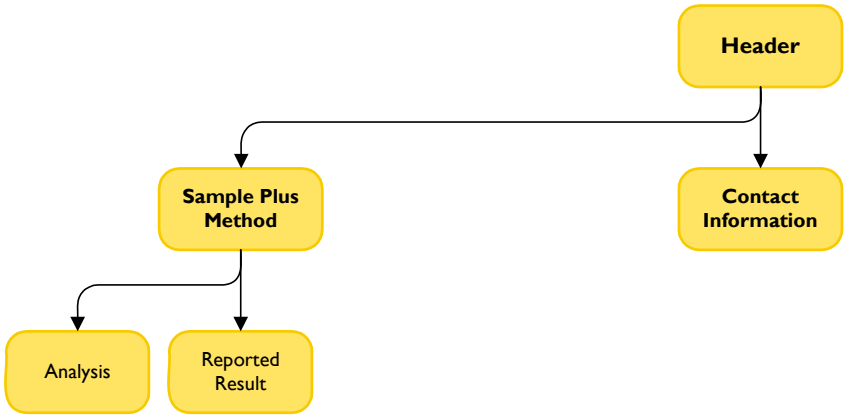
Definition: A measure of the success of the preparation part of the method as a percent.

Applicable Node(s):

Analysis For radiochemistry, the number of atoms of interest making it through sample preparation as a percentage of the number in the sample aliquot.

Appendix B
A Visual Representation of the Stages of SEDD (Figures)

Figure 1. SEDD Stage 1



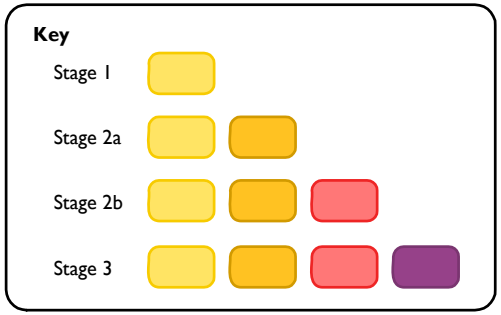


Figure 2. SEDD Stage 2a

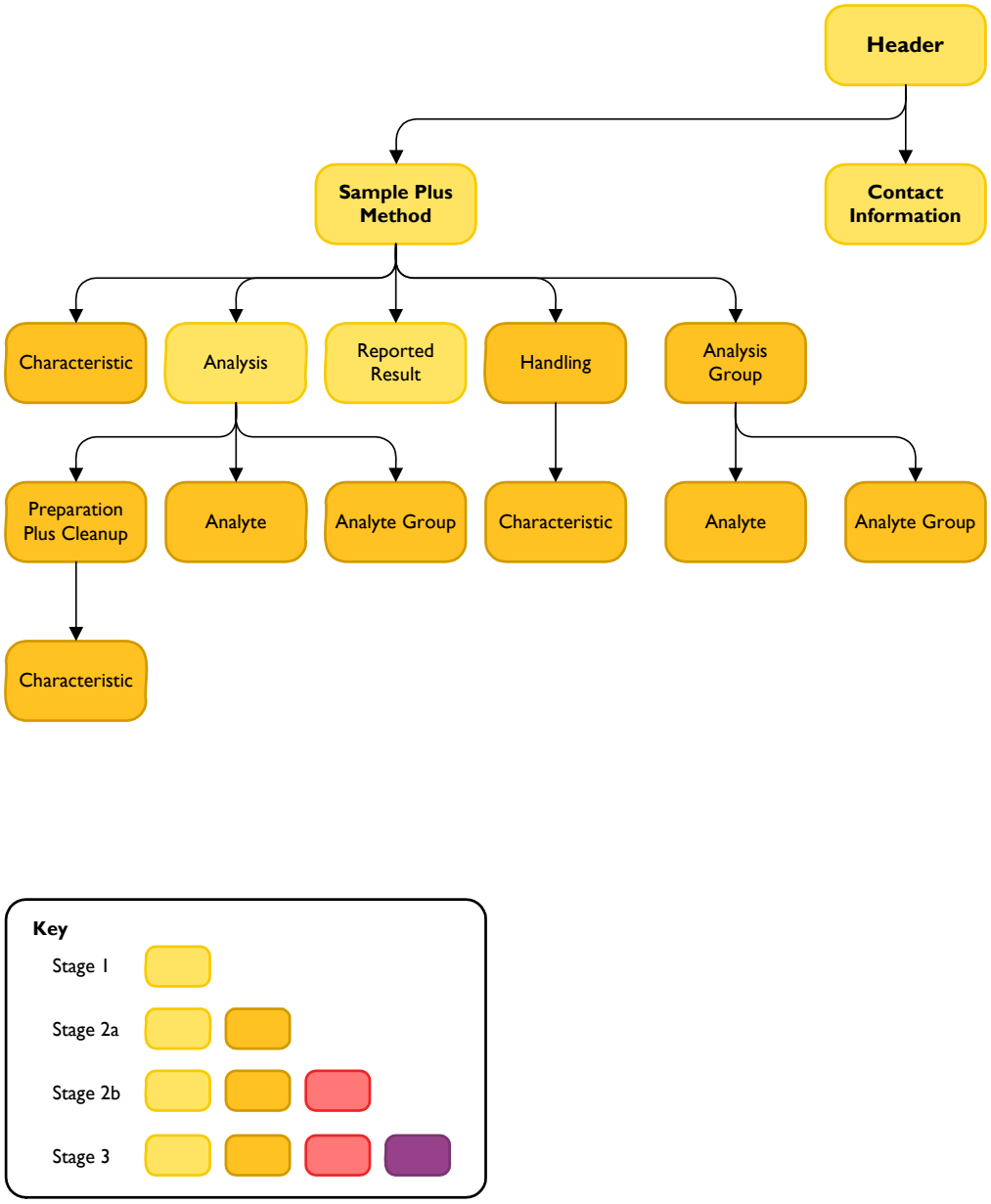


Figure 3. SEDD Stage 2b

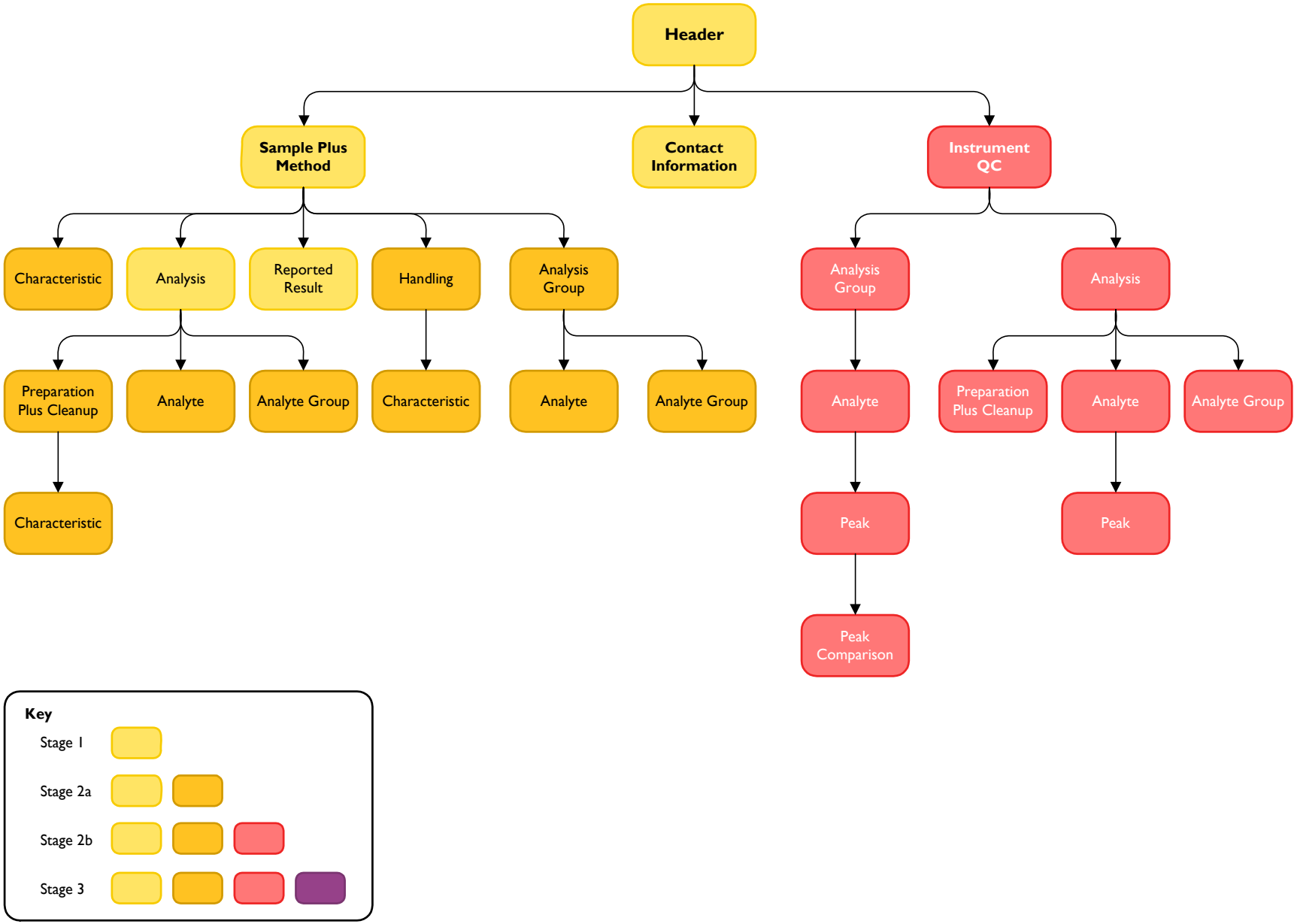
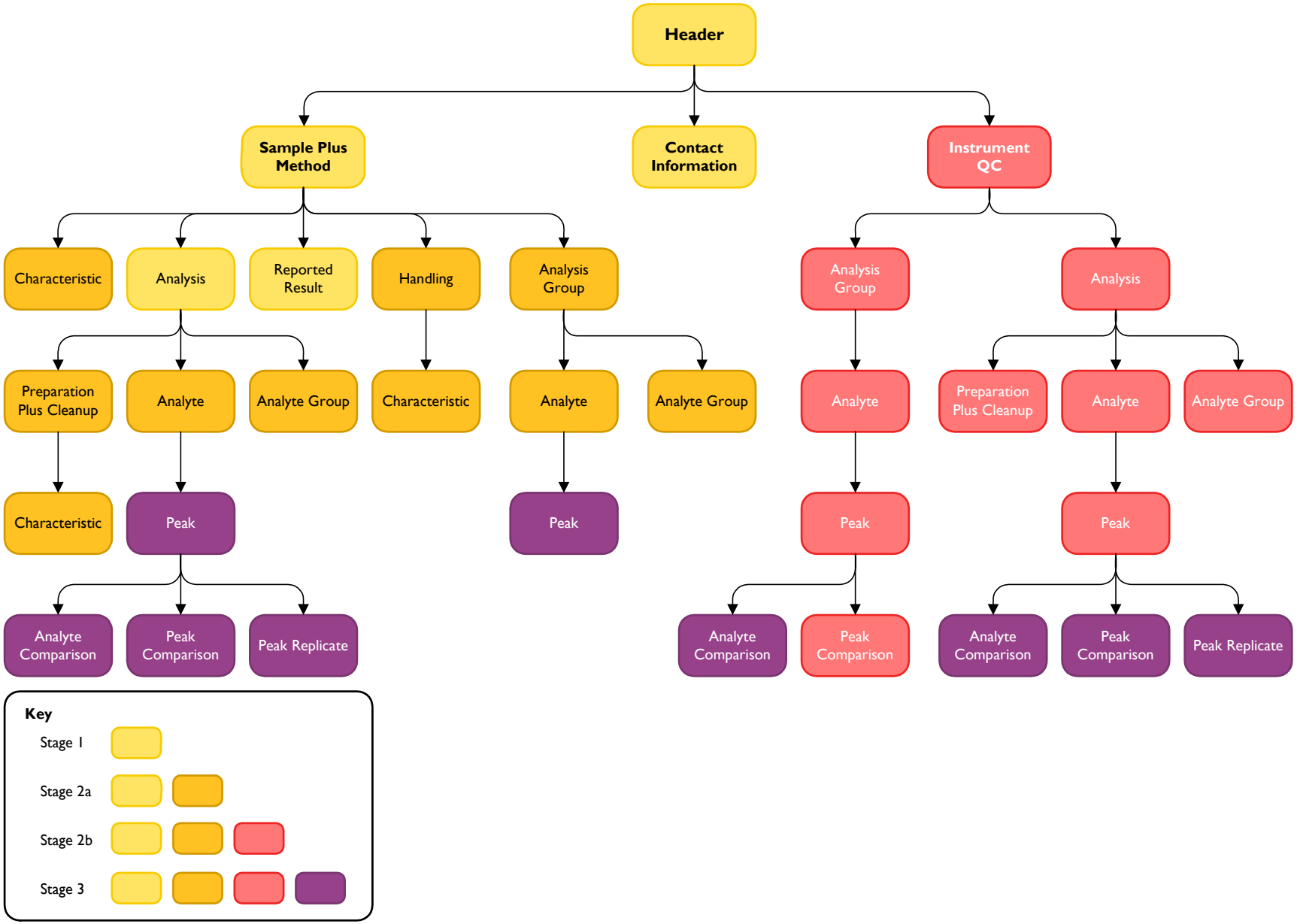


Figure 4. SEDD Stage 3



Appendix C
Glossary

The following terms are used throughout this document:

Data Element - A data element consists of a start tag, content, and an end tag. A data element may contain other elements. The SEDD Data Element Dictionary (DED) contains the list of data elements (tags) that developers may use. The SEDD Structure specifies relationships between certain elements from the DED.

Data Element Dictionary (DED) - The Data Element Dictionary contains the definitions of the defined data elements along with where in the structure they can be used.

Data Generator - Individual(s) or organization(s) directly responsible for generating data. For purposes of this document, the data generator is assumed to be the person or organization responsible for producing and transmitting the EDD to the data requester. Examples of Data Generators include analytical, radiological, or field laboratories.

Data Requester(s) - Individual(s) or organization(s) directly responsible for requesting analytical services and data from the analytical laboratory. For the purposes of this document, the data requester is assumed to be the person or organization responsible for developing the DTD or Schema and for developing the specific instructions for the resultant electronic data deliverable. Examples of Data Requesters include Federal or State Agencies, private engineering or environmental firms, etc.

DTD (Document Type Definition) - The DTD provides the set of rules for developing the structure and data elements for specific XML EDD formats. These rules are established by the data requester and the SEDD structure.

Electronic Data Deliverable (EDD) - An electronic file created by a data generator (usually the analytical laboratory) for transmitting and reporting analytical data.

Schema - The Schema (similar to but more powerful than the DTD) would give the set of rules for developing the structure and data elements for specific EDD formats along with the criteria for specifying the attributes of the data reported. These rules are established by the data requester and the SEDD structure.

SEDD Specification - A specification for developing standardized electronic data deliverable formats for environmental analytical data. Under this specification, a common structure and dictionary are required.

XML (eXtensible Mark-up Language) - This is a standard devised by the World Wide Web Consortium (W3C) and provides a common approach to representing information over the Web. XML is a language for describing data. It was developed as an extension to HTML (Hypertext Markup Language) for complex document creation and to provide a better vehicle for the transfer of information between databases. XML is not owned by any one vendor and thus remains an open standard. XML is text based, therefore it is processable using any platform. Data is transferred in SEDD as an XML document.