UNITED STATES DEPARTMENT OF DEFENSE

General Data Validation Guidelines

Environmental Data Quality Workgroup

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General Data Validation Guidelines

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General Data Validation Guidelines Change Sheet

1. Global change – All references to DoD Quality Systems Manual (QSM) version 5.1 have been updated to DoD Quality Systems Manual (QSM) version 5.3.

2. Section 2.0 Scope – The following text has been added to the end of the first paragraph:

“Data validation should not be confused with data usability. It is anticipated that project decisions will be supported by data usability determinations aided by the results of data validation.”

3. Section 3.0 Responsibilities – The following text has been added:

“It is anticipated that data validation is performed by a party independent of the laboratory. Project teams may identify a government quality assurance validation as necessary. A government quality assurance validation is defined as being independent of the prime contractor and performed by a government representative or services directly contracted by the government agency independent of the prime contractor.”

4. Section 4.1 Introduction – The following text has been removed from the fourth paragraph:

“Data validation should not be confused with data usability.”

The following text has been added to the fourth paragraph:

“Data validation is distinct from a data usability assessment.”

Contents

General Data Validation Guidelines

1.0 Purpose

This document provides guidance on the validation of environmental data generated in support of Department of Defense (DoD) projects, primarily from SW-846 methods. The entire DoD data validation guidance will be composed of this document plus analytical technique specific guidelines.

The objectives of the data validation and reporting procedures outlined in this guidance are to:

- Provide a clear understanding of the quality and limitations of the data using documented validation procedures;
- Encourage consistency in the way in which data are validated and reported for DoD projects; and
- Include items for Project Management consideration during the planning stages of a project.

Note: The analytical technique specific data validation guidelines will be published as separate modules.

2.0 Scope

This guidance can be applied to the validation of environmental data generated in support of DoD projects. This guidance applies primarily to chemical analytical data based on the requirements presented in the DoD Quality Systems Manual (QSM) version 5.3 and applicable SW-846 methods. This guidance is specific for data validators responsible for validating data for DoD. Data validation should not be confused with data usability. It is anticipated that project decisions will be supported by data usability determinations aided by the results of data validation.

This document serves as professional guidance for data validation and expands upon the protocols outlined in the Uniform Federal Policy-Quality Assurance Project Plan (UFP-QAPP) Manual (DoD/EPA 2005). This document is intended to provide the foundation for the validation process by providing guidance on validation procedures and report content.

Validation requirements as identified in a project-specific QAPP should always supersede the guidance of this document. The data validation guidelines presented in each project QAPP should be appropriate to the Data Quality Objectives (DQOs) of that project. The guidance provided in this document is not intended to obviate the need for professional judgment during the validation process. Professional judgment may be required in areas not fully addressed by this guidance document. Deviations from any validation procedure while planning or executing project activities should be documented in accordance with project requirements.

If the appropriate quality control documentation and information are provided and defined, this guidance may also be useful in labeling the scope and content of verification and

validation performed on analytical data generated by less traditional means such as field analytical methods (e.g., X-ray fluorescence, image analysis, immunoassay methods, or direct sensing). Information in this guidance may be utilized in the generation and presentation of the data reporting, data validation, and electronic data deliverable elements of specific Quality Assurance Project Plans (QAPPs). This guidance should be implemented by personnel familiar with the techniques and methodologies contained herein.

Refer to: *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods (SW-846), Update V, Chapter 1* and the *DoD/DOE Quality Systems Manual for Environmental Laboratories, version 5.3* for definitions of applicable terms.

3.0 Responsibilities

Data validation personnel are responsible for implementing these procedures for the validation of data and generation of validation reports. However, it is recognized that planning and proper establishment of validation requirements is necessary during the contracting phase as well as during the writing and approval of the QAPP. Project personnel (e.g., prime contractors, remedial project managers, and project chemists) are responsible for the scope and extent of validation for their projects.

It is anticipated that data validation is performed by a party independent of the laboratory. Project teams may identify a government quality assurance validation as necessary. A government quality assurance validation is defined as being independent of the prime contractor and performed by a government representative or services directly contracted by the government agency independent of the prime contractor.

4.0 Validation Steps

4.1 INTRODUCTION

This document outlines the validation of environmental data obtained under United States (US) DoD projects. The document incorporates other applicable elements of federal policies and guidance as noted in the references section. For example, this document incorporates conventional data validation language such as “stages of validation” previously developed (e.g., the USEPA Superfund program).

Based on the laboratory data deliverables and data validation requirements identified in the project QAPP, the analytical data may undergo “Stage 1” through “Stage 4” data validation or some combination of these. The extent of the data validation performed will be dependent on the project data quality objectives (DQOs) and will be limited by the content of the laboratory data deliverable. This procedure establishes guidance for the content of the validation reports and the validation process. The development of project DQOs is beyond the scope of this guidance.

Data validation should not be confused with compliance monitoring. Data validation is an explanatory process that extends the evaluation of data beyond method, procedural, or contractual compliance to determine the analytical quality of a specific data set. Data validation informs the user of any limitations on a data set and can identify project non-

compliance. However, enforcement of compliance is not within the authority of the data validator.

Data validation is distinct from a data usability assessment. Analytical data validation is the systematic review of laboratory data deliverables and can help identify laboratory and field sample analytical uncertainty. Data usability assessment also encompasses field sampling uncertainty including the overall sampling plan, sampling processes and conditions during sampling. A data validation report can be one element used during an assessment of the overall usability of the data. Data validation is an evaluation of data with respect to the project measurement quality objectives (MQOs), while data usability is an evaluation of the data with respect to the overall goals of the project as outlined in the DQOs.

It should be re-emphasized that it is not the role of data validation to determine if project goals have been met or to provide the decisions to be made. Data validation provides the overall appraisal of a data set and the project team should use this appraisal along with their own judgment when making decisions. It is not the role of data validation to accept or reject data. As such, the conventional R (reject) flag has been removed from this document. The project team should make the decision to accept or reject qualified data during the Data Usability stage, in accordance with the QAPP (for example, using the process described in UFP-QAPP Worksheet #37).

This document may also be used for guidance to indicate basic contractual validation requirements during the generation of project-specific QAPPs. Specifically, this document may be used as guidance to identify the required laboratory data deliverable, the extent of data validation to be performed, and the data validation qualifiers and reason codes to be used. These requirements should be included within the body of the QAPP or as appendices.

4.2 LABORATORY DATA DELIVERABLES

The types of laboratory data deliverables for each stage of data validation are intended to correspond as closely as possible to the stages of data validation outlined in *Guidance for Labeling Externally Validated Laboratory Analytical Data for Superfund Use* (USEPA 2009) and as defined in Appendix A of the *Quality Systems Manual ver. 5.3* (DoD/DOE 2019). The types of laboratory data deliverables per stage are as follows:

A Cover Sheet, Table of Contents, and Laboratory Case Narrative are required for all stages.

Stage 1: Sample results forms, chain of custody and supporting records (such as ground courier documents), laboratory receipt checklist, and field QC records (if separate from chain of custody).

Stage 2A: Includes all of **Stage 1** plus method QC (preparation batch QC) and forms. The following is a non-inclusive list:

- Sample related QC data and QC acceptance criteria linked to corresponding field samples (such as method blanks, matrix duplicates, surrogates, and serial dilutions);

- Requested spike analytes or compounds as appropriate (such as LCS, matrix spike, and surrogate recoveries, and post digestion spikes);

- QC sample frequency checked for appropriateness (for example, one LCS per twenty samples per 24 hours in a preparation batch).

Stage 2B: Includes all of **Stage 2A** plus instrument QC forms and preparation logs. The following is a non-inclusive list:

- Initial calibration summaries detailing the following: calibration type, individual standard concentrations, individual response factors, individual abundances, average response factors, correlation coefficients, and linear dynamic range results;

- Initial and continuing calibration verification summaries along with associated concentrations and percent recoveries or percent differences;

- Method specific forms such as tune and interference check summaries and internal standard summaries;

- All summary forms listed above for second column or detector including percent difference between the two analytical results;

- Preparation logs, including records supporting special techniques applied by the laboratory, such as Incremental Sampling Methodology (ISM) subsampling (included to allow evaluation of applicable quality control checks as detailed in the QAPP).

Stage 3: Includes all of **Stage 2B** plus instrument quantitation forms (raw data) necessary to recalculate sample results, method, and instrumentation QC; and standards traceability logs to include copies of vendor "Certificates of Analysis".[1]

Stage 4: Includes all of **Stage 3** plus all data (such as instrument chromatograms and spectra) necessary to qualitatively evaluate the results (for example, tentatively identified compound searches, all manual integration summaries with reasons, and evaluation of chromatographic baselines).

The extent of data validation that can be performed will be dependent upon the required type of laboratory data deliverable. For example, a Stage 3 data review cannot be performed without a Stage 3 or Stage 4 data deliverable. Successive stages of data validation require more comprehensive data deliverables from the laboratory. For example, Stage 1 data validation requires the review of sample receipt data from the laboratory, whereas Stage 4 requires all the outputs of the previous stages (Stage 1 through Stage 3) and evaluation of sample chromatograms and mass spectra. Therefore, Stage 4 data validation requires raw

[1] Standards traceability will allow recalculation of standards derived from primary stock concentration to working stock or spiking concentration and should be included in a Stage 3 data deliverable if the potential exists for legal chain of custody requirements during the project.

data (such as spectra) to evaluate results and cannot be performed on a deliverable containing only sample receipt forms.

4.3 ELEMENTS OF DATA VALIDATION

The process by which analytical data validation should be carried out depends on the stage assigned to that data type in the project QAPP. The assigned stage will be based on the DQOs required. The laboratory data should be delivered in a report that is, at a minimum, the same stage as the assigned stage of validation. The laboratory analytical data deliverable may be a hard copy deliverable, an electronic data deliverable, or a combination of both. The validator may validate the analytical data using entirely manual, entirely electronic, or a combination of both processes.

Data validators should document their findings in a report format that provides clear support and definition for the data qualifiers and reason codes applied. Data validators may also annotate sample result forms and EDDs with appropriate validation qualifiers and reason codes if required by the QAPP. The completed data validation reports may be sent either as a hard copy or an electronic file to the data recipient or customer. Examples of data validation reports and annotated sample result forms may be found in Appendices 4 and 5, respectively.

When the hardcopy of the report is validated, but a project EDD is used as the official data source for archival or storage, the project EDD should be compared to the hardcopy report to confirm that the results match. When performing part or full manual validation on a hardcopy (such as a pdf) report, a minimum of 10% of the sample results per method reported should be cross-checked against any project-required EDD. The data elements to be reviewed should be detailed in the project QAPP.

The steps in the process of staged data validation are outlined below.

(1) The analytical data package should be checked or verified by the data validator for *completeness* to ensure that all data requested are present in the data deliverable. The reporting requirements for the analytical data package should be specified in the QAPP. This is a critical step as analytical data validation may not be possible if any part of the requested laboratory data deliverable is not present. If any required data are missing, the point of contact (such as a remedial project manager or project chemist) should be notified to secure the missing data.

(2) The completeness check in step (1) should be followed by a QAPP *compliance* check to compare the documented sample receipt conditions and analytical QC results in the analytical data package to the requirements in the QAPP. The analytical QC results generally consist of two parts: (1) preparation batch QC, and (2) instrument-related QC. If the check is not in compliance with the QAPP, document this in the appropriate section of the data validation report. The point of contact should be notified about any preparation batch/analytical QC limits that are not consistent with QAPP requirements.

(3) The completeness and QAPP compliance checks may be followed by *recalculation checks*. This step is required only for Stage 3 and Stage 4 data validation and is dependent upon receipt of at least a Stage 3 laboratory data deliverable. The laboratory reported values

(e.g., sample results, instrument calibration result) can be checked by recalculating them using the data from instrument outputs reported by the laboratory. The objective is to ensure that the laboratory used proper calculations and procedures to determine the final reported values. This step may extend to other raw data, such as percent solids/moisture raw measurements from balances to assure dry basis calculations are correct. This step may be done on a fraction or percentage of instrument outputs, which should be specified in the QAPP. The QAPP should also specify that additional results should be recalculated and checked if any issues are noted with the first recalculated values.

(4) The *actual instrument outputs* such as chromatograms or spectra may be checked to ensure that the laboratory reported analytes have been correctly identified and quantitated. This step is required only for Stage 4 data validation and is dependent upon receipt of a Stage 4 laboratory data deliverable. This step also may be done on a fraction or percentage of instrument outputs which should be specified in the QAPP. The QAPP should specify that additional outputs should be checked if any issues are noted with the first fraction or percentage reviewed.

4.4 STAGED DATA VALIDATION

For the purposes of this guidance, the following terminology is recommended for use to describe the stages (extent) and processes used to validate laboratory analytical data packages, whether the validation is performed by a manual process, electronic process, or combination of both.

Note: The following lists of required activities per each stage of validation is not considered an “all inclusive” list or applicable to every method that is validated.

Stage 1: A verification and validation conducted only on completeness and compliance of sample specific information and field QC: field sample IDs and target analytes verified against the chain of custody for completeness; sample conditions upon arrival at laboratory noted; sample preservation was appropriate and verified by the laboratory; holding times were met; concentrations and units for limits of detection and quantitation were appropriate; trip blanks, field blanks, equipment blanks, and field duplicates met project requirements for frequency and field quality control.

Stage 2A: Stage 1 validation plus evaluation of preparatory batch QC results: method blanks, laboratory control samples, matrix spikes, laboratory duplicates (LCSD, MSD, DUP), surrogates (organics), serial dilutions, post digestion spikes (as appropriate to the method), and any preparatory batch cleanup QC to assure project requirements for analyte spike list, frequency, and quality control limits are met.

Stage 2B: Stage 2A validation plus evaluation of instrument-related QC results including Instrument Performance Samples: Tunes, breakdown standard check results, peak tailing factors (if applicable), instrument initial calibration summaries (including response factors and any regression summaries), initial calibration verification and continuing calibration verification summaries, internal standards, initial and continuing calibration blank summaries, confirmation of positive results for second column or detector including percent difference between the two analytical concentrations that are greater than the detection limit, and

interference check samples to assure project requirements for frequency and quality control criteria are met.

Stage 3: Stage 2B validation plus re-quantification and recalculation of selected samples (i.e., target analytes quantitated from appropriate internal standards) and instrument QC: Appropriate selection of curve fit type, weighting factors, and with or without forcing through zero, continuing calibration verifications and blanks, and percent ratios of tunes and performance checks including calculation of DDT/Endrin breakdown and column peak tailing, and preparatory batch QC results (such as spike percent recoveries and serial dilution percent differences) from instrument response. Instrument response data are required to perform re-quantification and recalculation.

Stage 4: Stage 3 validation plus qualitative review of non-detected, detected, and tentatively identified compounds (TICs) from instrument outputs: Chromatograms are checked for peak integration (10% of automated integration and 100% of manual integrations (MI) where chromatograms from before and after MI are examined for cause and justification), baseline, and interferences; mass spectra are checked for minimum signal to noise, qualitative ion mass presence, ion abundances; retention times or relative retention times are within method requirements for analyte identification. Raw data quantitation reports, chromatograms, mass spectra, instrument background corrections, and interference corrections are required to perform review of the instrument outputs.

Greater detail on the exact steps and processes to follow during Stages 3 and 4 of validation may be found in the following discussion of percentage data validation and in the validation guidelines for the individual methods/analytical technologies that follow this section of the guidelines.

Note: Using higher stages of data validation does not necessarily result in higher quality data. However, the quality of the analytical data becomes more transparent as more stages of validation are conducted, and the source of problems identified in lower stages of validation may be uncovered. Thus, the usability of the analytical data for its intended use becomes better understood.

Additionally, the generated data validation report should indicate, via use of the label codes listed below, the steps as well as the manner used for laboratory data verification and validation.

Label	**Corresponding Label Code**
Stage_1_Validation_Electronic	S1VE
Stage_1_Validation_Manual	S1VM
Stage_1_Validation_Electronic_and_Manual	S1VEM
Stage_2A_Validation_Electronic	S2AVE
Stage_2A_Validation_Manual	S2AVM

Label	Corresponding Label Code
Stage_2A_Validation_Electronic_and_Manual	S2AVEM
Stage_2B_Validation_Electronic	S2BVE
Stage_2B_Validation_Manual	S2BVM
Stage_2B_Validation_Electronic_and_ Manual	S2BVEM
Stage_3_Validation_Electronic	S3VE
Stage_3_Validation_Manual	S3VM
Stage_3_Validation_Electronic_and_Manual	S3VEM
Stage_4_Validation_Electronic	S4VE
Stage_4_Validation_Manual	S4VM
Stage_4_Validation_Electronic_and_ Manual	S4VEM
Not_Validated	NV

4.5 PERCENTAGE DATA VALIDATION IN STAGES 3 AND 4

When a Stage 3 or 4 manual data validation is performed, the requested re-quantifications and recalculations may be performed on a percentage of the samples in a project. The percentage can vary based on project needs to save time and money. When a Stage 3 or Stage 4 EDD is provided, an automated data validation at Stage 3 could be performed on 100% of the samples.

Note: It is understood that Stage 3 or 4 level validation cannot be fully automated with 100% success at this time. However, validators are still encouraged to attempt automated data validation on all their datasets regardless of Stage. The DoD encourages continued innovation in automated data review.

To encourage consistency in the interpretation of the percentage of re-quantifications and recalculations, the following guidelines were established as the minimum that should be performed, if required. If project requirements dictate any recalculation needs, those needs should be clearly defined in the QAPP. In cases where the QAPP defines requirements other than those below, the QAPP shall supersede this guidance.

Re-quantification and recalculation should be performed on the designated percentage of the samples per Sample Delivery Group (or however defined in the QAPP, such as percentage of total project samples) per analytical suite. As a minimum, it is recommended that 10% of the data should be re-quantified and re-calculated unless specific instructions are given in the QAPP.

When choosing samples, preparatory batch QC, and analytes for re-quantification and recalculation, consideration should be given to how samples are processed and analyzed to help assure a representative subsample of recalculations is performed. Additionally, if priority contaminants or contaminants of concern are identified in the QAPP, those analytes should be selected for re-quantification and recalculation. Other circumstances that should be prioritized for re-quantification and recalculation include samples that were diluted, target analytes that had manual integrations, and samples that were re-analyzed.

Initial calibration recalculations should use the raw instrument response for the target analytes and associated internal standards (if applicable) to recreate the calibration curve from the individual calibration standards. If multiple types of calibration curves are employed in an analytical suite, then one analyte per curve type should be recalculated. Re-quantification of instrument QC samples, preparatory batch QC samples, and sample results should use raw instrument response in tandem with the reported calibration factor, response factor, or slope; the preparation information; and percent moisture for solid samples to recreate the reported result. Instrument and preparatory batch QC sample recalculations should include verification of the percent recovery (%R), percent difference (%D), relative percent difference (RPD), or other reported data quality indicators. When a method requires dual column (confirmation) analysis, the same analyte should be recalculated from both columns and the reported RPD between columns verified.

Sample calculations should include the raw instrument result, re-quantified from the instrument response against the calibration function, and the final reported sample result, including any dilution, preparation factor, or percent moisture (if applicable). Surrogate results and recoveries should be re-quantified and recalculated where applicable. When no detects are present in the samples, re-quantification and recalculation of the surrogate (Stage 3) along with review of the chromatogram for absence of any analyte response (Stage 4) serves as verification of the sample quantification.

Any discrepancies or errors that are discovered during recalculation should trigger validators to consult their point of contact for further direction. If possible, the validator should try to determine if the errors are random or systematic. Errors of any sort may trigger more extensive recalculation (Stage 3), increased manual review of the instrument chromatography (Stage 4), and a request for a revised data deliverable from the laboratory. The scope of additional review triggered by errors or discrepancies should be clearly discussed in the data validation report and outcomes described in accordance with QAPP instructions.

Documentation of the Stage 3 for all recalculations performed, whether in the form of a checklist, handwritten calculations, or spreadsheet, should be included in the data validation report. An example of a recalculations spreadsheet is included in Appendix 6. Documentation of the Stage 4 re-interpretations, integrations, or other qualitative identification parameter should include the pages of the laboratory deliverable that were visually reviewed. Documentation of Stage 3 and Stage 4 validation performed via electronic means should include the identification of any automated data review software used and include the output report.

4.6 CONTENT AND FORMAT OF THE DATA VALIDATION REPORT

The data validation report should consist of the following major components. The presentation format of the information below is an example:

4.6.1 Cover Letter

The cover letter should contain the generation date of the cover letter, the address of the project office, the sample delivery group (SDG) number(s), the Project Manager's name or designee, name and address of the laboratory and laboratory contact, data validator's name and contact information, and applicable QAPP citation. The cover letter should list the specific data validation reports being sent with the cover letter. The cover letter may apply to data validation reports from more than one SDG. Appendix 2 is an example of the cover letter. The data validation report should be paginated in a manner such that on each page there is an identification to ensure that the page is recognized as a part of the report and there is a clear identification of the end of the report.

4.6.2 Data Validation Reports by SDG

Each SDG (however named) should be associated with a data validation report. The procedures used to generate the report(s) are discussed in the following sub-sections.

4.6.2.1 COVER PAGE AND INTRODUCTION

The cover page should indicate the SDG number(s) and analysis techniques/methods. The introduction should contain a brief description of the SDG information that is pertinent to data validation. This information includes the SDG title and number, Project Manager, the sample matrices and analyses performed on the samples, the data validation stage for the project, and a brief discussion of the methodologies/stages used for data validation. This section should also contain a Sample Identification Table listing each field sample identification number (as indicated on the field chain of custody) cross-referenced with its associated internal laboratory identification number and the validation stage performed. Each sample should be listed under every analytical method for which data were validated. Appendix 3 is an example of the sample identification table.

4.6.2.2 DATA VALIDATION FINDINGS

This section should present the data validation findings. The findings should be determined based on validation criteria established for each analytical technique as defined by the technique specific validation guidelines.

A discussion of each QC criteria and any applicable non-conformities under each analytical method should be presented in the data validation report for each analytical category.

4.6.2.3 DATA VALIDATION CHECKLISTS

A manual or electronic checklist for each analytical category listed above should be completed and should be included in the data validation report. The checklist may be defined in project planning documents or may be a standard or custom checklist. The checklist should address all QC elements for each analytical method in the report. It is recommended that the checklist be approved or included in the QAPP to ensure that all required aspects are

sufficiently addressed during the validation process. Examples of data validation checklists may be found in Appendix 4.

4.6.2.4 DOCUMENTATION OF RECALCULATIONS

Documentation of the recalculations performed during Stages 3 and 4 validation should be included in the data validation report. The documentation may be in the form of hand-written calculations, a verification generated during electronic validation, or a spreadsheet. An example of a calculations spreadsheet may be found in Appendix 6.

Note: All recalculations performed during Stages 3 and 4 validation can be provided in the validation report in the form of an appendix or addendum.

4.6.2.5 LABORATORY REPORTS (FORM ONES, SAMPLE RESULTS FORMS)

Annotated laboratory reports with the appropriate data qualifiers and qualification codes (if applicable), as specified in the data validation procedures, may be submitted as an appendix to the data validation report. Formats may include tabulated excel, word, or other EDD formatted files provided from the laboratory. Alternatively, an annotated data sheet (however named) with handwritten validation qualifiers may be submitted. An example is provided in Appendix 5.

4.6.3 Acronyms and Abbreviations List

This list should present all acronyms and abbreviations used in the individual data validation reports. Appendix 1 is an example of an acronyms and abbreviations list.

4.6.4 Data Qualifier Reference Table

Data qualifiers are applied in cases where the data do not meet the required quality control (QC) criteria or where special consideration by the data user is required. The data qualifiers that are recommended for use with these guidelines are listed in Section 4.8. Project needs may dictate the use of other data qualifiers. The data qualifiers to be used should be listed and defined in the QAPP, as well as, in the data validation report.

4.6.5 Qualification Code Reference Table

Qualification codes explain why data qualifiers have been applied and identify possible limitations and bias of data use. Appendix 7 provides an example of the qualification codes that may be used. Alternate or additional qualification codes may be specified in the project QAPP based on project needs. If required, qualification codes are to be provided by data validation personnel in the body of the data validation report on the annotated “certificates of analysis” provided by the laboratory.

4.6.6 EDDs

The stages of data validation defined in this document coincide with USEPA guidance on Electronic Data Deliverables (EDDs) such as Staged Electronic Data Deliverables (SEDD). Data validation may include a manual review of test reports, electronic data review (with data checkers), or a combination of both. A laboratory’s electronic data output should comply with the EDD data structure as outlined in the QAPP. A generic automated electronic data review checklist for SEDD Stage 2B can be located at the DoD DENIX/EDQW website.

Note: SEDD is used in a generic sense in this document for simplicity. It does not preclude the use of other Component file structures, such as Navy NEDD or Air Force ERPIMS.

4.7 RECOMMENDED RECALCULATIONS FOR STAGE 3 DATA VALIDATION

Calculations are performed in Stage 3 data validation. Stage 4 data validation additionally includes the qualitative evaluation of non-detect, detected, and tentatively identified analytes from instrument outputs. Specific guidance on the qualitative evaluation can be found in the individual analytical technique guidelines. The following manual calculations are included in Stage 3 or higher.

The QAPP may require more extensive recalculations. Requirements in the QAPP will always supersede this guidance.

A minimum of reported quality control calculations should be verified at a frequency of 10% per analytical method, per SDG. If the SDG is analyzed on multiple instruments, then each instrument should be included in the calculations. A minimum of 10% of the laboratory standards (instrument QC), field QC samples, field samples, and batch QC samples, should be undergo re-quantification, per analytical suite, per SDG. Project specific target analyte detects should also undergo re-quantification (minimum 10%) per analytical suite, per SDG. When choosing samples for re-quantification, precedence should be given to priority contaminants, diluted samples, manual integrations, and any samples requiring re-analysis.

When performing re-quantification on samples, instrument QC samples, and preparatory batch QC samples, the calculation should begin with the raw instrument response. Once the calibration curve is verified, as recommended below, the reported calibration factors may be used for re-quantification of other target analytes in the samples, instrument QC samples, and batch QC samples.

These recommendations were based on the National Functional Guidelines, adapted for SW-846 methods, and are not comprehensive for all methods. These recommendations should be adapted for methods that do not fall into one of the categories below.

If errors in the calculations are discovered, the validator should contact the project management team for further direction.

4.7.1 Organic Methods

Note: In this section, the term ‘target analyte’ is considered the same as project specific analytes of concern identified in the project QAPP.

4.7.1.1 GAS AND LIQUID CHROMATOGRAPHY (GC AND LC)

Note: these calculations include SW-846 methods such as: PCBs (8082), pesticides (8141), herbicides (8151), PAHs (8310), and nitroaromatics (8330).

Samples

Re-quantify all the target analyte detects for at least 10% of the samples in each SDG. Include dilution, prep factors, and percent moisture to recalculate the reported result.

Re-quantify all detects found in the field QC blanks (such as field blanks or equipment blanks).

Note: If no samples in the SDG contain detects, the surrogate recalculation may serve as verification of sample results.

If the method requires confirmation of detects on a second detector or analytical column, re-quantify analytical results for both primary and secondary for all detects. Verify both concentrations are greater than the detection limit as directed by the QAPP and both peaks from each column fall within their retention time windows.

Preparatory Batch QC

Laboratory Control Sample (LCS):

Re-quantify the result and recalculate the percent recovery for at least 10% of the target analytes per each LCS.

Surrogates:

Re-quantify the surrogate result and recalculate percent recovery for at least 10% of the samples. If more than one surrogate was used, vary the surrogate compound to have approximately the same number of manually re-quantified concentrations and manual recalculations of percent recoveries per surrogate compound.

Matrix Spike/Matrix Spike Duplicate (MS/MSD) or LCS Duplicate:

Re-quantify the spike result concentration and recalculate percent recovery and relative percent difference (RPD) for at least 10% of the target analytes in each MS/MSD sample pair.

Method Blank:

Re-quantify one or more detects found in the method blank (if applicable), per each SDG.

Instrument QC

GC Column Performance:

Ensure no calculation errors occurred by recalculating 10% of the injection port inertness checks (if applicable) reported on summary forms for DDT or Endrin. Review tailing factors for GC column performance as required by the specific analytical technique or in accordance with QAPP instructions.

Initial Calibration:

Recalculate the initial calibration for at least 10% of the target analytes from each initial calibration proportionally selecting analytes based on calibration curve types used and for each internal standard (if applicable).

Average Relative Response Factor ($\overline{RRF}$):

Recalculate individual RRFs, $\overline{\mathrm{RRF}}$, and the percent relative standard deviation (%RSD) for target analytes selected from each internal standard. Include all second column/detector positive detects.

Average Calibration Factor ($\overline{CF}$):

Recalculate individual CFs, $\overline{CF}$, and the percent relative standard deviation (%RSD).

Linear or Quadratic Regression:

Recalculate the slope, intercept, and correlation coefficient.

Relative Standard Error (RSE):

If the initial calibration included refitting the data back to the model (RSE), then recalculate 10% of the target analytes from each initial calibration for the RSE.

Initial and Continuing Calibration Verification (ICV/CCV):

Re-quantify and recalculate the initial and continuing calibration verifications for at least 10% of the target analytes for every ICV/CCV proportionally selecting analytes based on calibration curve types used in the initial calibration. The target analytes should be based upon on project QAPP analytes of concern.

RRF:

Re-quantify ICV/CCV concentrations to verify reported values on the associated summary forms for target analytes selected from each internal standard.

Recalculate the ICV/CCV RRF and percent difference (%D) from the average RRF for target analytes selected from each internal standard.

CF:

Re-quantify the ICV/CCV concentrations to verify reported values on the associated summary forms.

Recalculate the ICV/CCV CF and percent difference (%D) from the average CF.

Linear or Quadratic Regression:

Re-quantify the ICV/CCV concentrations to verify reported values on the associated summary forms.

Recalculate the ICV/CCV calibration factor and percent drift from the average calibration factor.

4.7.1.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY (GC/MS)

Note: these calculations include SW-846 methods such as: volatiles (8260), semi-volatiles (8270), and dioxins/furans (8290).

Samples

Re-quantify all the target analyte detects for at least 10% of the samples in each SDG. Include dilution, prep factors, and percent moisture (if applicable) to recalculate the reported result.

Re-quantify all detects found in the field QC blanks (such as trip blanks, field blanks or equipment blanks).

Note: If no samples in the SDG contain detects, the surrogate recalculation may serve as verification of sample results.

Preparatory Batch QC

LCS:

Re-quantify the result and recalculate the percent recovery for at least 10% of the target analytes per each LCS.

Surrogates:

Re-quantify and recalculate percent recoveries for all surrogate results in the 10% of samples and method QC that were originally selected.

MS/MSD (or LCS Duplicate):

Re-quantify the spike result concentration and recalculate percent recovery and relative percent difference (RPD) for at least 10% of the target analytes in each MS/MSD sample pair.

Method Blank:

Re-quantify one or more detects found in the method blank (if applicable), per each SDG.

Instrument QC

GC Column Performance and Injection Port Inertness /Tune:

Ensure no calculation errors occurred by recalculating 10% of the abundance ratios and the percent degradation of DDT in every tune, and recalculate the peak tailing factor (if applicable). Ensure tune criteria specified by the analytical method or QAPP are met.

Initial Calibration:

Recalculate the initial calibration for at least 10% of the target analytes per each internal standard per each initial calibration proportionally selecting analytes based on calibration curve types used.

Average Relative Response Factor ($\overline{RRF}$):

Recalculate individual RRFs and $\overline{\mathrm{RRF}}$ for target analytes from each internal standard.

Recalculate the percent relative standard deviation (%RSD) for these target analytes per each internal standard.

Linear or Quadratic Regression:

Recalculate the slope, intercept, and correlation coefficient.

Initial and Continuing Calibration Verification (ICV/CCV):

Re-quantify and recalculate the initial and continuing calibration verifications for at least 10% of the target analytes proportionally per each internal standard for every ICV/CCV proportionally selecting analytes based on calibration curve types used in the initial calibration.

RRF:

Re-quantify ICV/CCV concentrations to verify reported values on the associated summary forms.

Recalculate the ICV/CCV RRF and percent difference (%D) from the average RRF.

Linear or Quadratic Regression:

Re-quantify the ICV/CCV concentrations to verify reported values on the associated summary forms.

Recalculate the ICV/CCV calibration factor and percent drift from the average calibration factor.

Relative Standard Error (RSE):

If the initial calibration included refitting the data back to the model (RSE), then recalculate 10% of the target analytes from each initial calibration for the RSE.

The following recalculations should be performed in addition to those listed above for GC/MS if High Resolution for dioxins, furans and PCB's are required:

Toxicity Equivalency Quantity/Factor (TEQ/TEF):

Recalculate at least 10% of the TEQ/TEF.

Estimated Detection Limit (EDL)/Estimated Maximum Possible Concentration (EMPC):

Verify at least 10% of the quantitated EDL concentrations.

Include EMPC results in the 10% of target analytes recalculated and re-quantified, if reported.

4.7.2 Inorganic Methods

Note: In this section, the term 'target analyte' is considered the same as project specific analytes of concern identified in the project QAPP.

4.7.2.1 WET CHEMISTRY

Note: these calculations include SW-846 methods such as: mercury (7470/7471), hexavalent chromium (7196/7197/7199), cyanide (9010), and anions (9056).

Samples

Re-quantify all the target analyte detects for at least 10% of the samples in the SDG. Include dilution, preparation factors, and percent moisture to recalculate the reported result.

Re-quantify all detects found in the field QC blanks (such as field blanks or equipment blanks).

Preparatory Batch QC

LCS:

Re-quantify the result and recalculate the percent recovery for at least 10% of the target analytes per each LCS (as applicable).

MS/MSD:

Re-quantify the spike result and recalculate percent recovery and relative percent difference (RPD) for at least 10% of the target analytes in each MS/MSD pair (as applicable).

Laboratory Duplicate:

Recalculate the RPD of all target analyte detects in each laboratory duplicate.

Note: Laboratory duplicates recalculation may not be applicable depending on the method or QAPP QC requirements.

Method Blank:

Re-quantify one or more detects found in the method blank (if applicable), per each SDG.

Instrument QC

Initial Calibration:

Linear or Quadratic Regression:

Recalculate the slope, intercept, and correlation coefficient for at least 10% of the target analytes in each initial calibration.

Initial and Continuing Calibration Verification (ICV/CCV):

Linear or Quadratic Regression:

Re-quantify the ICV/CCV concentrations to verify reported values on the associated summary forms for at least 10% of the target analytes in each calibration verification.

Recalculate the ICV/CCV calibration factor and percent drift from the average calibration factor for at least 10% of the target analytes in each calibration verification.

4.7.2.2 INDUCTIVELY COUPLED PLASMA (ICP-AES) AND MASS SPECTROMETRY (ICP-MS)

Note: these calculations include SW-846 methods such as: metals by ICP-AES (6010) and metals by ICP-MS (6020).

For ICP-AES and ICP-MS instrumentation, the calibration algorithms vary widely among manufacturers. For this reason, the recalculation of ICP-AES and ICP-MS initial calibrations may produce results that do not match those reported by the laboratory. The validator must be provided with the instrument specific algorithm necessary to perform the recalculation. In cases where the algorithm cannot be obtained, the validator must use professional judgment in the evaluation of the calibration curve. The manufacturer of the instrument is expected to comply with SW-846 inorganic method requirements.

Samples

Re-quantify all the target analyte detects for at least 10% of the samples in the SDG. Include dilution, prep factors, and percent moisture to recalculate the reported result.

Re-quantify all detects found in the field QC blanks (such as field blanks or equipment blanks).

Preparatory Batch QC

LCS:

Re-quantify the result and recalculate the percent recovery for at least 10% of the target analytes per each LCS.

MS/MSD:

Re-quantify the spike result and recalculate percent recovery and relative percent difference (RPD) for at least 10% of the target analytes in each MS/MSD pair.

Laboratory Duplicate:

Recalculate the RPD for at least 10% of the target analytes in each laboratory duplicate.

Note: Laboratory duplicates recalculation may not be applicable depending on the method or QAPP QC requirements.

Method Blank:

Re-quantify one or more detects found in the method blank (if applicable), per each SDG.

Serial Dilution:

Recalculate the percent difference for at least one target analyte.

Post Digestion Spike:

Recalculate one post digestion spike per SDG for at least 10% of the target analytes.

Instrument QC

Mass Calibration (ICP-MS Tune):

Ensure no calculation errors occurred by recalculating 10% of the average mass and %RSD for every tune.

Initial Calibration:

Recalculate the initial calibration for at least 10% of the target analytes per each initial calibration, proportionally selecting analytes based on calibration curve types used.

Linear or Weighted-linear Regression:

Recalculate the slope, intercept, and correlation coefficient.

Relative Standard Error (RSE):

If the initial calibration included refitting the data back to the model (RSE), then recalculate 10% of the target analytes from each initial calibration for the RSE.

Initial and Continuing Calibration Verification (ICV/CCV) and Low-Level Calibration Verification (LLCCV):

Re-quantify and recalculate the ICV, CCV, and LLCCV for at least 10% of the target analytes for every ICV, CCV, and LLCCV proportionally selecting analytes based on calibration curve types used in the initial calibration.

RRF:

Re-quantify ICV/CCV concentrations to verify reported values on the associated summary forms for target analytes from each internal standard.

Recalculate the ICV/CCV RRF and percent difference (%D) from the average RRF for these target analytes from each internal standard.

Verify the LLCCV result and recalculate percent recovery.

Linear or Weighted-linear Regression:

Re-quantify the ICV/CCV concentrations to verify reported values on the associated summary forms.

Recalculate the ICV/CCV calibration factor and percent drift from the average calibration factor.

Verify the LLCCV result and recalculate percent recovery.

Interference Check Samples:

Verify the result and recalculate the percent recovery for at least 10% of the target analytes for every interference check standard. Recalculate at least 10% of the reported concentrations of non-spiked metals in each ICS.

4.8 DATA VALIDATION QUALIFIERS

The following provides a brief explanation of the DoD data validation qualifiers assigned to results during the data review process by a data validator. The reviewer should use these qualifiers, as applicable, unless other data qualifiers are specified in a project related document, such as a QAPP. If other qualifiers are used, a complete explanation of those qualifiers should accompany the data validation report.

Qualifier	Definition
U	The analyte was not detected and was reported as less than the LOD or as defined by the customer. The LOD has been adjusted for any dilution or concentration of the sample.
J	The reported result was an estimated value with an unknown bias.
J+	The result was an estimated quantity, but the result may be biased high.
J-	The result was an estimated quantity, but the result may be biased low.
N	The analysis indicates the presence of an analyte for which there was presumptive evidence to make a "tentative identification."
NJ	The analyte has been “tentatively identified” or “presumptively” as present and the associated numerical value was the estimated concentration in the sample.
UJ	The analyte was not detected and was reported as less than the LOD or as defined by the customer. However, the associated numerical value is approximate.
X	The sample results (including non-detects) were affected by serious deficiencies in the ability to analyze the sample and to meet published method and project quality control criteria. The presence or absence of the analyte cannot be substantiated by the data provided. Acceptance or rejection of the data should be decided by the project team (which should include a project chemist), but exclusion of the data is recommended.

Note: R (reject) flag has been removed; see Section 4.1

5.0 Records

Data validation record retention requirements for hard copies and electronic formats should be defined in the QAPP for the project. At a minimum, data validation records should be retained the same length as the original laboratory report (i.e., 5 years or as specified by the QAPP).

6.0 References

The following documents were reviewed in the preparation of the DoD Data Validation Guidelines:

2005. *Uniform Federal Policy for Quality Assurance Project Plans, Part 1: UFP-QAPP Manual*. *Final Version 1.* Intergovernmental Data Quality Task Force (IDQTF). DoD: DTIC ADA 427785, EPA-505-B-04-900A. March. On-line updates available at: http://www.epa.gov/fedfac/pdf/ufp_qapp_v1_0305.pdf.

2019. *Department of Defense/Department of Energy Consolidated Quality Systems Manual for Environmental Laboratories Version 5.3* DoD Environmental Data Quality Workgroup and DOE Consolidated Audit Program (DOECAP).

2014. *Test Methods for Evaluating Solid Waste, Physical/Chemical Methods, SW-846.* 3rd ed., Update V, Revision 2. Environmental Protection Agency, United States (EPA). Office of Solid Waste. July.

2011. *USEPA National Functional Guidelines for Chlorinated Dibenzo-p-Dioxins (CDDs) and Chlorinated Dibenzofurans (CDFs) Data Review.* EPA-540-R-11-016. (OSWER 9240.1-53). Office of Superfund Remediation and Technology Innovation (OSRTI). September.

2016. *USEPA National Functional Guidelines for High Resolution Superfund Methods Data Review*. EPA-542-B-16-001. (OLEM 9200.3-115). Office of Superfund Remediation and Technology Innovation (OSRTI). April.

2014. *USEPA National Functional Guidelines for Inorganic Superfund Data Review.* USEPA-540-R-013-001. (OSWER 9355.0-131). Office of Superfund Remediation and Technology Innovation (OSRTI). August.

2014. *USEPA National Functional Guidelines for Superfund Organic Methods Data Review.* USEPA-540-R-014-002. (OSWER 9335.0-132). Office of Superfund Remediation and Technology Innovation. August.

2009. *Guidance for Labeling Externally Validated Laboratory Analytical Data for Superfund Use.* EPA 540-R-8-005 (OSWER 9200-1-85). Office of Solid Waste and Emergency Response. January.

2005. *Guidance for Evaluating Performance-Based Chemical Data*. EM200-1-10. Department of the Army, US Army Corps of Engineers. June.

2008. *SEDD Specifications Document & Data Element Dictionary Version 5.2.* USEPA Contract Laboratory Program. July.

2013. *SEDD Valid Values Document Version 1.0.* USEPA Contract Laboratory Program. May.

7.0 Attachments

Appendix 1: Example Acronyms and Abbreviations

Appendix 2: Example Sample Cover Letter

Appendix 3: Example Sample Identification Table

Appendix 4: Example Data Validation Reports & Checklists

Appendix 5: Example Annotated Laboratory Data Sheets

Appendix 6: Example Calculations Spreadsheet for Stage 3

Appendix 7: Example Qualification Code Reference Table

Appendix 1: Example Acronyms and Abbreviations

Appendix 1: EXAMPLE ACRONYMS AND ABBREVIATIONS

Following is a list of acronyms and abbreviations that may be used in data validation reports:

%D	percent difference
%R	percent recovery
%RSD	percent relative standard deviation
$\overline{CF}$	average calibration factor
$\overline{RRF}$	average relative response factor
CCB	continuing calibration blank
CCV	continuing calibration verification
DL	detection limit
DQO	data quality objective
ICAL	initial calibration
ICB	initial calibration blank
ICS	interference check sample
ICV	initial calibration verification
IS	internal standard
LCS	laboratory control sample
LD	laboratory duplicate
LLCV	low-level calibration verification
LOD	limit of detection
LOQ	limit of quantification
MB	method blank
MS	matrix spike
MSD	matrix spike duplicate
QAPP	quality assurance project plan

RPD relative percent difference

RT retention time

SD sample duplicate

SDG sample delivery group

TEQ toxicity equivalency quantity

TIC tentatively identified compound

Appendix 2: Example Sample Cover Letter

Appendix 2: Example Sample Cover Letter

(Date)
(Project Manager or
Designee) (Company
address)

Dear ( ):

Enclosed is Revision __ of the data validation reports for project (number) from Work Plan/QAPP Title (number) as follows: Semi-volatiles SDG S0221 SDG S0350 by SW-846 Method 8270D, laboratory reports (A and B); Pesticides/PCBs SDG S0201 by SW-846 Methods 8081B/8082, laboratory report (C); and Metals SDG S0221 SDG S0201 by SW-846 Method 6010B, laboratory report (D and E). The SDGs were analyzed by (laboratory name, address). The laboratory project manager is (name, contact info). The specific sample identifications are listed in the Sample Identification Table(s). The data packages were reviewed according to the *DoD General Data Validation Guidelines version1, 2018*.

(List data validation references)

Sincerely,

(Signature)

Data Validation Project Manager (Data Validator)
Contact information

Appendix 3: Example Sample Identification Table

Appendix 3: Example Sample Identification Table

Client Sample ID	Laboratory Sample ID	Matrix	Validation Stage
FB-BS04-E01-D10.0	2720-1	water	S4VEM
FB-BS04-B01-D10.0	2720-2	water	S2BVE
FB-BS04-B02-D10.0	2720-3	water	S2BVE
FB-SS01-S01-D0.5	2720-4	soil	S2BVEM
FB-BS01-S01-D10.0	2720-5	soil	S3VEM
FB-SS02-S01-D0.5	2720-6	soil	S2BVEM
FB-BS02-S01-D10.0	2720-7	soil	S2BVEM
FB-BS02-D01-D10.0	2720-8	soil	S2BVEM
FB-SS03-S01-D0.5	2720-9	soil	S2BVEM
FB-BS03-S01-D10.0	2720-10	soil	S2BVEM

Appendix 4: Example Data Validation Reports and Checklist

Note: The following are just example validation reports and checklists. They may not comply with your specific project and should not be used as specified (for example, “cut and paste” into your documents). It is expected that each validation group will develop their own validation reports and checklists consistent with project objectives.

EXAMPLE Data Validation Report A

Site Name: Site AXA

Collection Date: March 22, 2012

Report Date: March 29, 2012

Matrix: Water

Parameters: Volatiles

Validation Stage: S4VM

ADR Software Identification: N/A

Laboratory and Report Number/Date: Laboratory B, report (X) on March 25, 2012

Sample Delivery Group (SDG): 1203308

Client Sample ID	Laboratory Sample ID
W	1203308-1
X	1203308-2
Y	1203308-3
Z	1203308-6
Trip Blank	1203308-7

Introduction
This data review covers three water samples, one equipment blank, and one trip blank listed above including dilutions and reanalysis as applicable. The analyses were performed by EPA SW 846 Method 8260B for Volatiles applying DoD QSM requirements.

This review follows the Master Quality Assurance Project Plan for Project A and the DoD General Data Validation Guidelines.

A qualification summary table is provided at the end of this report if data have been qualified.

The following are definitions of the data qualifiers (from the QAPP).

Qualifier	Definition
U	The analyte was not detected and is reported as less than the LOD or as defined by the customer. The LOD has been adjusted for any dilution or concentration of the sample.
J	The reported result is an estimated value (e.g., matrix interference was observed, or the analyte was detected at a concentration outside the calibration range).
J+	The result is an estimated quantity, but the result may be biased high.
J-	The result is an estimated quantity, but the result may be biased low.
N	The analysis indicates the presence of an analyte for which there is presumptive evidence to make a "tentative identification."
NJ	The analyte has been "tentatively identified" or "presumptively" as present, and the associated numerical value is the estimated concentration in the sample.
UJ	The analyte was not detected and is reported as less than the LOD or as defined by the customer. However, the associated numerical value is approximate.
X	The sample results (including non-detects) were affected by serious deficiencies in the ability to analyze the sample and to meet published method and project quality control criteria. The presence or absence of the analyte cannot be substantiated by the data provided. Acceptance or rejection of the data should be decided by the project team (which should include a project chemist), but exclusion of the data is recommended.

Note: R (reject) flag not used.

Sample Receipt

All sample receipt documentation was complete and correct. No anomalies were noted.

Holding Time/Preservation

The samples were analyzed within the technical holding times and were properly preserved.

GC/MS Instrument Performance Check

The instrument performance check met frequency and ion abundance requirements.

Initial Calibration

The initial calibration was performed using the correct number of standards at appropriate concentrations.

The percent relative standard deviations (%RSDs) were ≤20% with the following exceptions. The coefficients of determination (r^2) were ≥0.995 for all compounds calibrated using linear regression or quadratic regression.

The %RSD for acetone, bromoform and 2-butanone were 22%. All associated sample results were non-detects and were not qualified.

Continuing Calibration

Percent differences (%Ds) between the initial calibration RRFs and the initial calibration verification (ICV) RRFs were ≤20%.

Continuing calibration verification (CCV) analysis was performed at the correct frequency.

Percent differences (%Ds) between the initial calibration RRFs and the CCV RRFs were ≤20%.

The ICV and CCV RRFs met all QC acceptance criteria.

Blanks

The method blank and trip blank met all QC acceptance criteria with the following exception:

Toluene was detected in the trip blank at a concentration > the limit of detection (LOD) but ≤ the limit of quantification (LOQ). All associated sample results were non-detects and were not qualified.

Surrogate Spikes

Surrogates were added to all field and QC samples. All surrogate percent recoveries were within QC acceptance limits.

Matrix Spike (MS)/Matrix Spike Duplicates (MSD)

The MS and MSD analyses met all QC acceptance criteria for percent recovery and relative percent difference (RPD) with the following exceptions:

The percent recoveries for MS (38%) and MSD (41%) for iodomethane were less than the laboratory lower control limit (70%), but ≥10%. The associated sample results were non-detects and were **qualified UJ**.

Laboratory Control Sample (LCS)

The LCS analysis met all QC acceptance criteria.

Internal Standards

The internal standard areas and retention times were within QC acceptance limits.

Target Compound Identification

All target compound identifications were within validation criteria for relative retention times, characteristic ions, and relative ion abundances.

Limits of Detection (LODs), Limits of Quantification (LOQs) and Reporting Limits (RLs)

All LODs, LOQs and RLs met project decision limits. The LODs for the non-detects and the LOQs for the detects were less than the action levels.

Tentatively Identified Compounds (TICs)

TICs were not reported in this SDG.

Field Duplicates

A field duplicate was not performed for this SDG.

Calculation Checks

The calculations for initial and continuing calibration select sample results for the samples noted above, LCS, MS, MSD, surrogate percent recoveries and RPDs, and confirmation RPDs were checked (10% of samples). No discrepancies were noted.

Overall assessment of Data

The overall assessment of data was acceptable. Data qualifiers are summarized in the following table.

Client Sample ID	Analyte	Qualifier	Qualification Code Reference
W	Iodomethane	UJ	M3
X	Iodomethane	UJ	M3
Y	Iodomethane	UJ	M3
Z	Iodomethane	UJ	M3
Trip Blank	Iodomethane	UJ	M3

Example Data Validation Checklist A	
SDG: 1203308	**Laboratory Sample ID: 1203308-1, -2, -3, -6, -7**
Method/Batch Number: 8260/VL120326-3	

Note only Outliers. Tune/Instrument Performance Check:

Frequency:√	**Ion Abundances:**√	

ICAL and Blanks:

Analyte	*ICAL RRF (>0.05)	ICAL %RSD (≤20%) or r^2(≥0.990)	ICV/CCV Frequency (12 hours)	*(ICV)/CCV RRF (>0.05)	(ICV)/CCV %D (≤20%)	Method Blank	Trip Blank	5X (10X) Blank
Acetone	√	22	√	√	√	√	√	NA
2-Butanone	√	22	√	√	√	√	√	NA
Bromoform	√	22	√	√	√	√	√	NA
Toluene	√	√	√	√	√	√	3.8	(38)

**Comments/Notes ***see Method for minimum RRFs

Sample	IS percent recovery (-50 to +100%)	IS RT +/-30s from ICAL mid-point	Sample	IS percent recovery (-50 to +100%)	IS RT +/-30s from ICAL mid- point
√	√	√	√	√	√

Batch QC

Analyte	LCS %R	MS %R	MSD %R	MS/D or LCS/D RPD	
Iodomethane	√	62	60	√	

Comments/Notes: LCS/MS/MSD laboratory limits. FD RPD 30% for W, 50% for soils.

Sample	Surr %R	Surr %R	Sample	Surr %R	Sample	Surr %R	Surr %R
None.	None.	None.	None.	None.	None.	None.	None.

EXAMPLE DATA VALIDATION REPORT AND CHECKLIST B

8260B VOCs

Laboratory SDG: **Chemist/Verifier:**

Associated Batches: **Contractor Program Chemist (CPC):**

Date Verified: **Date CPC review:**

Client: **Project Title:**

Laboratory:

Guidance: DoD Guidelines for Data Review and Validation Version 1

Applicable QAPP:

ADR Software Identification: **Company ADR 2, Version 3**

Sample ID #	Sample Date	Date Lab Received	Date Analysis Run	Methods	Validation Label Code
A	3/3/15	3/4/15	3/7/15	8260B	S3VEM
B	3/3/15	3/4/15	3/7/15	8260B	S3VEM
C	3/3/15	3/4/15	3/7/15	8260B	S3VEM
D	3/3/15	3/4/15	3/7/15	8260B	S3VEM
E	3/3/15	3/4/15	3/7/15	8260B	S3VEM

Note: “Yes/No” answers that indicate a possible data quality issue are shaded. If answer falls in the shaded area, an explanation must be provided below each applicable question box. Also include if any discussion occurred with the project chemist for discussion or concurrence.

Laboratory Case Narrative

Verification Criteria	Yes	No	N/A
Were any DoD QSM deviations noted in the laboratory case narrative?		X	
Were DoD QSM corrective actions followed if deviations were noted?			X
Were any issues noted in the cooler receipt form?		X	

Sample Documentation

Verification Criteria	Yes	No
Were all samples documented correctly on the chain-of-custody (COC)?	X	
Did samples listed on COCs match the sample labels?	X	
Were samples relinquished properly on the COC?	X	
Were all samples properly preserved?	X	
Were all samples analyzed within the specified holding times?		X

Samples X, Y, and Z were received and analyzed beyond the HT but within 2X the HT. All associated sample results that were detects were qualified J and non-detects were qualified UJ.

Instrument Performance Check (Tuning) ([1] list instrument ID, date and time tune was run.) (Manual / Electronic)

Verification Criteria for instrument_____[1]	**Yes**	**No**
Was instrument tune check completed prior to calibration?	X	
Was instrument tune check completed every 12 hours during sample analysis?	X	
Were ion relative abundance for each target mass within the required intensities limits listed in the Table of SW-846 8260?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was instrument tune check completed prior to calibration?	X	
Was instrument tune check completed every 12 hours during sample analysis?	X	
Were ion relative abundance for each target mass within the required intensities limits listed in the Table of SW-846 8260?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was instrument tune check completed prior to calibration?	X	
Was instrument tune check completed every 12 hours during sample analysis?	X	
Were ion relative abundance for each target mass within the required intensities limits listed in the Table of SW-846 8260?	X	

Initial Calibration ([1] list instrument ID, date and time tune was run.)

Verification Criteria for instrument_____[1]	**Yes**	**No**
Was at least a 5-point calibration completed for all analytes prior to sample analysis?	X	
Was lowest standard at or below the LOQ?	X	
Are the average response factors (RFs) above the minimum response factor? ($\geq$0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, $\geq$0.1 for chloromethane, bromoform, and 1,1- dichloroethane.)	X	

Verification Criteria for instrument_____[1]	**Yes**	**No**
Are the RSDs for RFs for CCCs % (vinyl chloride, 1,1-dichloroethene, chloroform, 1,2-dichloropropane, toluene, and ethylbenzene) ≤30% and one option below?	X	
Option 1: RSD for each analyte ≤ 20%?	X	
Option 2: If linear least squares regression was used, was the r ≥ 0.995?	X	
Option 3: If non-linear regression was used, was the coefficient of determination r^2 ≥0.99?	X	
If non-linear regression was used, were 6 points used for second order and 7 points for third order?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was at least a 5-point calibration completed for all analytes prior to sample analysis?	X	
Was lowest standard at or below the LOQ?	X	
Are the average response factors (RFs) above the minimum response factor? (≥0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, ≥0.1 for chloromethane, bromoform, and 1,1- dichloroethane.)	X	
Are the RSDs for RFs for CCCs % (vinyl chloride, 1,1-dichloroethene, chloroform, 1,2-dichloropropane, toluene, and ethylbenzene) ≤ 30% and one option below?	X	
Option 1: RSD for each analyte ≤ 20%?	X	
Option 2: If linear least squares regression was used, was the r ≥ 0.995?	X	
Option 3: If non-linear regression was used, was the coefficient of determination r^2 ≥0.99?	X	
If non-linear regression was used, were 6 points used for second order and 7 points for third order?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was at least a 5-point calibration completed for all analytes prior to sample analysis?	X	
Was lowest standard at or below the LOQ?	X	

Verification Criteria for instrument_____[1]	**Yes**	**No**
Are the average response factors (RFs) above the minimum response factor? (≥0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, ≥0.1 for chloromethane, bromoform, and 1,1- dichloroethane.)	X	
Are the RSDs for RFs for CCCs % (vinyl chloride, 1,1-dichloroethene, chloroform, 1,2-dichloropropane, toluene, and ethylbenzene) ≤ 30% and one option below?	X	
Option 1: RSD for each analyte ≤ 20%?	X	
Option 2: If linear least squares regression was used, was the r ≥ 0.995?	X	
Option 3: If non-linear regression was used, was the coefficient of determination r^2 ≥ 0.99?	X	
If non-linear regression was used, were 6 points used for second order and 7 points for third order?	X	

Initial Calibration Verification [(ICV) Second Source] ([1] list instrument ID, date and time tune was run.)

Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the ICV confirmed as a second source and analyzed after each calibration?	X	
Was the ICV %difference (%D) for all analytes within ±20% of the expected value (initial source)?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the ICV confirmed as a second source and analyzed after each calibration?	X	
Was the ICV %difference (%D) for all analytes within ±20% of the expected value (initial source)?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the ICV confirmed as a second source and analyzed after each calibration?	X	
Was the ICV %difference (%D) for all analytes within ±20% of the expected value (initial source)?	X	

Continuing Calibration Verification (CCV) ([1] list instrument ID, date and time tune was run.)

Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the CCV analyzed daily before sample analysis?	X	
Was the CCV analyzed every 12 hours of analysis time and following the last sample?	X	
Are the average response factors (RFs) above the minimum response factor? (VOCs -≥0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, ≥0.1 for chloromethane, bromoform, and 1,1- dichloroethane).	X	
Was the CCV %difference (%D) or %Drift for VOCs within ±20% and ±50% for the ending CCV?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the CCV analyzed daily before sample analysis?	X	
Was the CCV analyzed every 12 hours of analysis time and following the last sample?	X	
Are the average response factors (RFs) above the minimum response factor? (VOCs -≥0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, ≥0.1 for chloromethane, bromoform, and 1,1-dichloroethane).	X	
Was the CCV %difference (%D) or %Drift for VOCs within ±20% and ±50% for the ending CCV?	X	
Verification Criteria for instrument_____[1]	**Yes**	**No**
Was the CCV analyzed daily before sample analysis?	X	
Was the CCV analyzed every 12 hours of analysis time and following the last sample?	X	
Are the average response factors (RFs) above the minimum response factor? (VOCs -≥0.30 for SPCCs chlorobenzene and 1,1,2,2- tetrachloroethane, ≥0.1 for chloromethane, bromoform, and 1,1- dichloroethane).	X	
Was the CCV %difference (%D) or %Drift for VOCs within ±20% and ±50% for the ending CCV?	X	

Internal Standard (IS) Recoveries

Verification Criteria (Applied to each batch and each instrument)	Yes	No
Were internal standards reported for all samples and standards?	X	
Were internal standard areas within -50% to + 100% of the ICAL midpoint standard area (or daily CCV)?	X	
Were retention time ± 30 seconds (or ±10 seconds for QSM requirements) from the retention time of the midpoint standard of the ICAL (or daily CCV)?	X	

Method Blank

Verification Criteria	Yes	No
Was one method blank run per method batch?	X	
No analytes were detected > 1/2 the LOQ or > 1/10 the amount measured in any sample or 1/10 the regulatory limit or common lab contaminants (methylene chloride, 2-butanone, and acetone) were < the LOQ?	X	
Did blank results affect sample results?	X	

LCS

Verification Criteria	Yes	No
Was a complete target analyte list of LCS including surrogates reported?	X	
Was one LCS run per preparatory batch?	X	
Were all percent recoveries within limits specified in the QAPP?	X	

Matrix Spike and Matrix Spike Duplicate

Verification Criteria	Yes	No
Was one MS and MSD run per preparatory batch per matrix?	X	

Verification Criteria	Yes	No
Were all MS percent recoveries within LCS control limits and also within project specified limits?	X	
Was the RPD between MS and MSD ≤20%?	X	

Surrogates

Verification Criteria	Yes	No
Were surrogates added to all field and QC samples?	X	
Were surrogate recoveries within the laboratory or project specified control limits?	X	

Field QC

Verification Criteria	Yes	No
Was a trip blank shipped with and analyzed with the samples in this SDG?	X	
Was the trip blank clean (No analytes were detected > 1/2 the LOQ or > 1/10 the amount measured in any sample or 1/10 the regulatory limit or common lab contaminants (methylene chloride, 2-butanone, and acetone) were < the LOQ)?	X	
Did blank results affect sample results?	X	
Were other field blanks collected and analyzed with the samples in this SDG?	X	
If so, were they clean (no analytes were detected > 1/2 the LOQ or > 1/10 the amount measured in any sample or 1/10 the regulatory limit or common lab contaminants (methylene chloride, 2-butanone, and acetone) were < the LOQ)?	X	
Did field blank results affect sample results?	X	
Were field duplicates or triplicates analyzed with the samples in this SDG?	X	
If so, did the duplicate (or triplicate) results meet QC acceptance criteria specified by the project (QAPP)?	X	

Sensitivity

Verification Criteria	Yes	No	N/A
Was the laboratory sensitivity consistent with project (QAPP) requirements?	X		
Did all analytes meet sensitivity requirements?	X		

Samples that have quantitation limits that do not meet QAPP requirements, based on dilutions, are listed in the table below.

Field ID	Parameter	Dilution
N/A	N/A	N/A

Target Compound Identification

Verification Criteria	Yes	No	N/A
Were the RRTs for detected compounds within 0.06 RRT units of the daily CCV?	X		
Do the relative intensities of the characteristic ions agree within ±30% of the relative intensities in the reference spectrum?	X		

Tentatively Identified Compounds

Verification Criteria	Yes	No	N/A
Were TICS requested with this SDG?	X		
Were the major ions present in the reference spectrum also present in the sample spectrum?	X		
Did the relative intensities of the major ions in the sample spectrum agree within ±20% of the reference spectrum?	X		

Additional Qualifications

Were additional qualifications applied or professional judgment used?

Field ID	Analyte	New RL	Qualification
None.	None.	None.	None.

Completeness

Verification Criteria	Yes	No	N/A
Were any data X qualified during the verification process?		X	
Were any samples lost, broken, or in any other manner in not verified?		X	
Were all requested sample analyses requested performed, the correct analyte lists used and correct sample preparation and analyses methods and units utilized?	X		

EXAMPLE C: EXAMPLE AUTOMATED DATA REVIEW CHECKLIST

Data Review QC	Checklist Item	Checklist Item	Yes	No	NA	Comment
2B	1	Did chain of custody information agree with the laboratory report?				
2B	2	Were samples preserved properly and received in good condition?				
2B	3	Were holding times met?				
2B	4	Were all requested target analytes reported?				
2B	5	Was the initial calibration within acceptance criteria?				
2B	6	Were CCVs at the proper frequency and within acceptance criteria?				
2B	7	Was a method blank prepared and analyzed for each batch?				
2B	8	Were target analytes in the method blank less than the LOD?				
2B	9	Were target analytes in the field blank less than the LOD?				
2B	10	Were LCS/LCSD recoveries within project specified limits?				
2B	11	Were MS/MSD recoveries within project specified limits?				
2B	12	Were MS/MSD RPDs within project specified limits?				
2B	13	Were surrogate recoveries within project specified limits?				
2B	14	Did any field duplicates meet the required RPD for the project?				
2B	15	Were project required laboratory PQLs achieved?				
2B	16	Have all Case Narrative findings been addressed?				

Appendix 5: Example Annotated Laboratory Data Sheet

GC/MS Volatiles

Method SW8260B

Sample Results

Lab Name: The Best Labs, Inc
FC Work Order Number: 321123
Client Name: Alpha and Omega Works
ClientProject ID: Far from Golgotha

Field ID: MW01
Lab ID: 321123-01

Analysis ReqCode: VOC

Sample Matrix: WATER
% Moisture: N/A
Date Collected: 20-Jun-16
Date Extracted: 22-Jun-16
Date Analyzed: 22-Jun-16
Prep Method: SW5030 Rev C

Prep Batch: V321123-3
QCBatchID: V321123-3-1
Run ID: V321123-3A
Cleanup: NONE
Basis: As Received
File Name:321123.D

Analyst: Andrea Sansom
Sample Aliquot: 10 ml
Final Volume: 10 ml
Result Units: UG/L
Clean DF: 1

CASNO	Target Analyte	Dilution Factor	Result	LOQ/LOD	DL	Laboratory Qualifier	Validation Qualifier
75-01-4	VINYL CHLORIDE	1	0.5	0.5	0.3	U	UJ
75-35-4	1,1-DICHLOROETHENE	1	0.5	0.5	0.3	U	UJ
156-60-5	TRANS-1,2-DICHLOROETHENE	1	0.5	0.5	0.3	U	UJ
156-59-2	CIS-1,2-DICHLOROETHENE	1	0.5	0.5	0.3	U	UJ
79-01-6	TRICHLOROETHENE	1	2.5	0.5	0.3		J-
127-18-4	TETRACHLOROETHENE	1	42	0.5	0.2		J-

Surrogate Recovery

CASNO	Surrogate Analyte	Result	Flag	Spike Amount	Percent Recovery	Control Limits
460-00-4	4-BROMOFLUOROBENZENE	20.1		25	80*	85 - 115
1868-53-7	DIBROMOFLUOROMETHANE	23.9		25	96	84 - 118
2037-26-5	TOLUENE-D8	23.8		25	95	85 - 115

Data Package ID: *321123-1*

Appendix 6: Example Stage 3 Calculation Spreadsheet

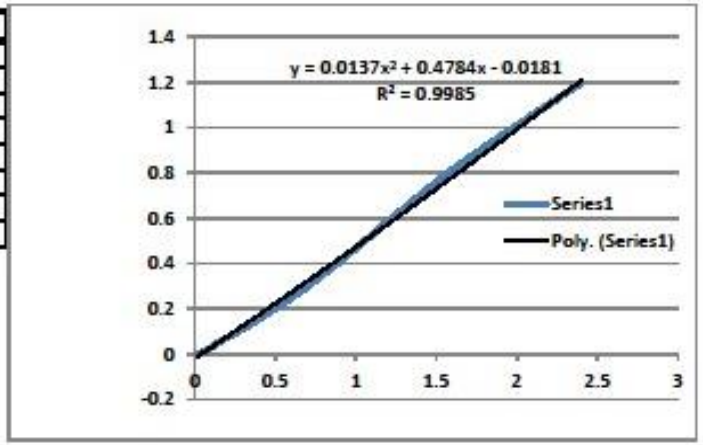
Example

VOCs Calculations for SDG 1311368

Calibration: Instrument A 6/21/10

ICAL Quadratic

Conc.	FBZ	Iodomethane	$Y=C_s/C_{is}$	$X= R_s/R_{is}$
0.5	2212987	8476	0.02	0.003830117
1	2179007	18973	0.04	0.008707177
2	2169676	45188	0.08	0.020827073
4	2166381	123726	0.16	0.057111838
10	2047255	320179	0.4	0.156394294
20	2162924	764685	0.8	0.353542242
40	2131127	1733522	1.6	0.813429702
60	2159552	2586644	2.4	1.197768796



	CCV 11/21/13
Surrogate	DBF
Int. Std. Response	1993477
Analyte Response	582774
Analyte Concentration	25
Int. Std. Concentration	25
CCRF	0.292
Conc. (ug/L)	25.7523
Ave RF	0.2838
CCV %D	3.0

coefficients	
a	0.0137
b	0.4784
c	-0.0181

	Iodomethane
Int. Std. Response	1993477
Analyte Response	250207
Analyte Concentration	10
Int. Std. Concentration	25
CCRF	NA
Conc. (ug/L)	7.44
Ave RF	NA
CCV %D	-25.6

Example

VOCs Calculations for SDG 1311368

Calibration: Instrument A 6/21/10

Average RF

				Chloromethane		Toluene		1,1,2,2-TCA	
Conc.	FBZ	CBZ-d5	DCBZ-d4	Area	RRF	Area	RRF	Area	RRF
0.5	2212987	867599	734605	22897	0.517	52396	3.020	15941	1.085
1	2179007	860308	728214	43515	0.499	100250	2.913	32005	1.099
2	2169676	855279	716303	85495	0.493	198769	2.905	61882	1.080
4	2166381	861120	729137	191539	0.553	434086	3.151	135938	1.165
10	2047255	807329	696003	379527	0.463	952207	2.949	319317	1.147
20	2162924	864940	741103	800911	0.463	1982998	2.866	641767	1.082
40	2131127	850067	722468	1655867	0.486	4066080	2.990	1284039	1.111
60	2159552	857925	737662	2319641	0.448	5861481	2.847	1898332	1.072
Multiplier				1		1		1	
AveRF				0.4902		2.9549		1.1052	
RSD				6.90		3.33		3.07	

	ICV	CCV 11/20/13	CCV 11/21/13
Surrogate	DBF	Tol-d8	4-BFB
Int. Std. Response	2137784	836570	641648
Analyte Response	609083	1842882	651923
Analyte Concentration	25	25	25
Int. Std. Concentration	25	25	25
CCRF	0.285	2.203	1.016
Conc. (ug/L)	25.0981	24.8769	25.8291
Ave RF	0.2838	2.2138	0.9834
CCV %D	0.4	-0.5	3.3
	Bromomethane	Bromoform	Hexachlorobutadiene
Int. Std. Response	2137784	836570	641648
Analyte Response	260724	148388	89814
Analyte Concentration	10	10	10
Int. Std. Concentration	25	25	25
CCRF	0.305	0.443	0.350
Conc. (ug/L)	9.7944	9.7524	10.4085
Ave RF	0.31130	0.45470	0.33620
CCV %D	-2.1	-2.5	4.1

Example

VOCs Calculations for SDG 1311368

	MB VL 131120	MB VL 131121	LCS VL 131120	LCS VL 131121	-4	-4MS	-4MSD	-4
Dilution/DF	1	1	1	1	1	1	1	10
Final Volume (mL)	5	5	5	5	5	5	5	5
Sample Aliquot (mL)	5	5	5	5	5	5	5	5
Surrogate	DBF	DBF	Tol-d8	Tol-d8	4-BFB	4-BFB	4-BFB	4-BFB
Internal STD Response	2038951	2014204	836570	812477	640838	638300	638331	558138
Surr Response	582912	585410	1842882	1766537	659521	670856	651490	602398
Calibration R.F.	0.2838	0.2838	2.2138	2.2138	0.9834	0.9834	0.9834	0.9834
Surr spike Conc. (ug/L)	25	25	25	25	25	25	25	25
Surr spike Conc. (ug/L)	25	25	25	25	25	25	25	25
Surr Conc. (ug/L)	25.184	25.603	24.877	24.553	26.163	26.719	25.946	27.438
Surr %REC	101	102	100	98	105	107	104	110
Analyte	MeCl	MeCl	4-M-2-Pentanone	1,3-DCP	trans-1,2-DCE	trans-1,2-DCE	trans-1,2-DCE	TCE
Internal STD Response	2038951	2014204	2116818	812477	2050628	2032082	1971123	1983454
TC Response	12775	26330	996083	370807	20424	250625	242622	90588
Calibration R.F.	0.4155	0.4155	0.28	1.1028	0.31180	0.31180	0.31180	0.2928
TC Conc. (ug/L)	0.3770	0.7885	42.0140	10.3462	0.7986	9.8889	9.8892	3.8996
Final Conc (ug/L)	0.37698	0.78853	42.01400	10.34618	0.79858	9.88988	9.88916	38.99577
		%R	84.03	103.46		90.90	90.71	
						0.20		

Appendix 7: Example Qualification Code Reference Table

Example Qualification Code Reference Table

Explanation of Infraction	Reason Code
Chemical Preservation Infraction	P1
Temperature Infraction	T1
Holding Time Infraction, Sampling to Analysis	H1
Holding Time infraction, Sampling to Extraction	H2
Holding Time Infraction, Extraction to Analysis	H3
Performance Evaluation Sample/Tune Infraction	P2
Resolution Check Infraction	R1
Initial Calibration Frequency Infraction	I1
Initial Calibration- Insufficient Number of Standards	I2
Initial Calibration RRF Infraction	I3
Initial Calibration %RSD, r or r^2 Value Infraction	I4
ICV/CCV Frequency Infraction	C1
ICV/CCV RRF Infraction	C2
ICV/CCV Infraction with High Bias	C3
ICV/CCV Infraction with Low Bias	C4
ICB/CCB Frequency Infraction	B1
ICB/CCB Infraction (Qualified Detect)	B2
ICS Frequency Infraction	I5
ICS A Infraction (Qualified Detect)	I6
ICS AB Infraction with High Bias	I7
ICS AB Infraction with Low Bias	I8
Internal Standard Infraction with High Bias	I9
Internal Standard Infraction with Low Bias	I10
Internal Standard RT Infraction	I11
Required Sample Cleanup not Performed	R2
Method Blank Frequency Infraction	B3
Method Blank Infraction (Qualified Detect)	B4
LCS Frequency Infraction	L1
LCS percent recovery Infraction with High Bias	L2
LCS percent recovery Infraction with Low Bias	L3
LCS/LCSD Duplicate precision infraction	L4
MS/MSD Frequency Infraction	M1
MS/MSD percent recovery Infraction with High Bias	M2

Explanation of Infraction	**Reason Code**
MS/MSD percent recovery Infraction with Low Bias	M3
MS/MSD or Duplicate Precision Infraction	M4
Post Digestion Spike infraction	M5
Surrogate percent recovery Infraction with High Bias	S1
Surrogate percent recovery Infraction with Low Bias	S2
Serial Dilution Infraction	S3
Confirmation Analysis not Performed	C5
Confirmation Precision Infraction	C6
Sample RT or RRT Infraction	R3
Spectral Match Infraction	S4
Ion Mass Ratio Criteria Infraction	I12
Result Exceeds Calibration Range	R4
Storage Blank Infraction (Qualified Detect)	B5
Trip Blank Infraction (Qualified Detect)	B6
Field Blank Infraction (Qualified Detect)	B7
Equipment Blank Infraction (Qualified Detect)	B8
Field Duplicate Precision Infraction	D1
Reporting Limit Exceeds Action Level	R5
Professional Judgment (include references to support basis of decision)	P3