Chapter 2
CHEMISTRY DATA REPORTING REQUIREMENTS AND DATA PACKAGE DELIVERABLES

2-1. Data Reporting Requirements. The chemistry data package should contain enough information to demonstrate that the project's DQOs have been fulfilled. In general, one should be able to determine the precision, accuracy, representativeness, comparability, and sensitivity of the data from information contained in the data package. This description applies to both primary and QA laboratory packages. The amount of information required to demonstrate attainment of DQOs depends upon the acceptable level of uncertainty for the intended data use. In general, the type of data package required will fall into one of three general categories.

a. Screening Data Package. Screening data are generated by methods of analysis that tend to be relatively rapid, are performed in the field (as opposed to an off-site laboratory), and have less rigorous sample preparation. Screening data provide analyte ID, but tend to report false positives. Their ability to quantitate analytes is in general less precise and less accurate than "definitive" type methods (see below). Screening data must be confirmed by sending at least 10% of the samples for definitive analysis.

(1) The screening data package will depend on the screening method used. A typical screening data package will include the following:

- sample ID number
- preparation method
- analysis method
- detection limits
- identity and quantity of analyte(s) present
- date and time of sample collection
- date of sample analysis
- field equipment calibration

(2) More sophisticated field screening methods will involve QC samples such as duplicate samples, calibration standards, spiked samples, and/or blank samples. Results for these associated QC samples should also be included in the screening data package.

b. Definitive Data Package. Definitive data are produced using rigorous analytical methods, such as EPA reference methods. Analyte presence and quantitation are confirmed through extensive QC procedures at the laboratory, which may be on-site or off-site. The definitive data package should include a cover sheet; Table of Contents; case narrative; the analytical results; sample documentation information; and internal laboratory QC/QA information. The data package should have sequentially numbered pages.

(1) Cover Sheet. The cover sheet should specify the following information:

- name and location of laboratory
- contract number
- project name & site location
- statement of data authenticity and official signature of release

(2) Table of Contents. Laboratory data packages should be organized in a format that allows for easy ID and retrieval of information. An index and/or table of contents should be included for this purpose.

(3) Case Narrative. A case narrative should be included in each report, outlining any problems with analysis. The case narrative should also list all methods used. The case narrative should contain a table correlating field sample numbers and laboratory sample numbers, and indicate which analytical test methods were performed and by which laboratories. Samples that were received but not analyzed should also be identified. Extractions or analyses that are performed out of holding times should be appropriately noted. The case narrative should define all data qualifiers or flags. Deviations of QC sample results from laboratory acceptance limits should be noted and associated corrective actions taken by the laboratory should be addressed. Any other factors that could affect the sample results (*e.g.*, air bubbles in VOC sample vials, excess headspace in soil VOC containers, the presence of multiple phases, inappropriate sample temperature, pH, container type or volume, *etc.*) Should be discussed.

(4) Analytical Results. The results for each sample should contain the following information at a minimum:

- project name and unique ID number
- field sample ID number as written on custody form
- laboratory name and location (city and state)
- laboratory sample ID number
- preparation and analysis batch numbers
- date sample collected
- date sample received
- date sample extracted or prepared
- date sample analyzed
- analysis time when holding time limit is less than forty-eight hours
- method numbers for all preparation and cleanup procedures
- analysis procedure including method numbers
- analyte or parameter
- detection limits (DL) - Estimated sample detection limits based on method detection limits adjusted for sample-specific factors (*e.g.*, aliquot size, dilution or concentration

factors, moisture content of a soil or sediment)
- quantitation limits (QL)
- analytical results with correct number of significant figures (Results for solid matrices should be reported on a dry weight basis)
- concentration units
- dilution factor: All reported data shall reflect any dilutions and/or concentrations. The dilution factor, if applicable, should be noted on the analytical report. If dilution is required for organic analytes, data from both runs should be recorded and reported.
- matrix (soil, water, oil, *etc*.)
- percent moisture or percent solids
- chromatograms, as needed
- sample aliquot analyzed
- final extract volume
- sample preservation

(5) Lower Limit Reporting. The laboratory may use a reporting limit (RL) expressed in terms of DL, QL, regulatory action level, or project-specific threshold limit, however the laboratory's use of these terms must be well defined. In addition, if the non-detect "ND", "U" ,"<", or other lower limit reporting convention is used, then these terms must also be defined.

(6) Sample Documentation. Original CoC record, shipping documents, and sample cooler receipt forms should be attached to each data package.

(7) QC/QA Information. The minimum data package must include internal laboratory QC/QA data with their respective acceptance criteria. The data package should also include the laboratory's method detection limits for project-specific parameters. The data package should correlate the method QC data with the corresponding environmental samples on a per batch basis. Method QC data include all spike recoveries, including surrogate spike recoveries; all measures of precision, including relative percent difference (RPD); and all control limits for accuracy and precision. This would include laboratory performance information such as results for method blanks (MBs), recoveries for Laboratory Control Standard (LCS) and Laboratory Control Standard Duplicate (LCSD), RPD for LCS/LCSD pairs, and recoveries for QC sample surrogates; and matrix-specific information such as sample duplicate RPDs, MS and MSD recoveries, MS/MSD RPDs, and field sample surrogate recoveries, serial dilutions, and post-digestion spikes. At a minimum, internal QC samples should be analyzed and reported at rates specified in the specific methods or as specified in the contract, whichever is greater. Any deviations from the control limits should be noted. For example, the data package should document the matrix spike(MS) and duplicate spike level, the MS and duplicate spike sample result, the percent recovery of the MS and duplicate, the respective RPD, and the acceptance criteria for spike recovery and RPD.

c. Comprehensive Data Package. A comprehensive data package contains sufficient information to completely reconstruct the analyses that were performed. Hence, comprehensive data packages include all batch QC results, instrument QC results (*e.g.*, initial calibration verification and continuing calibration verification), method detection limit studies, and raw data (*e.g.*, run logs, sample preparation logs, standard preparation logs, and printed instrumental output such as chromatograms). Typically, comprehensive data packages are required if third-party data validation is to be performed. EPA national functional guidelines, EPA regional functional guidelines, and project-specific guidelines for validation may all have distinct reporting formats. The appropriate validation guidelines should be consulted to determine what type of data package is required.

2-2. Data Reporting Format. Definitive data should be reported as hard copy and electronic deliverables with no discrepancies between the two. It is recommended that hard copy data reports and electronic data deliverables be generated from the same electronic database. Hard copy analytical data should be reported using a standard format.

2-3. Data Package Deliverable Time Schedule. A schedule for data delivery should be established so that data packages are provided as needed for chemical QA assessment.

2-4. Sample Identification Table. The sample ID table is used to provide the CMQAL with the necessary sample ID information for preparation of the CQAR. The sample ID table correlates field sample numbers and laboratory sample numbers. It relates field, QC, and QA samples to one another where the relationship is not obvious, and identifies field QC samples (*i.e.*, trip blanks (TBs), equipment blanks (EBs), background samples) where their identity has been concealed. See Table 2-1 for an example table format.

Table 2-1
Sample Identification Table

Project Name and Number:_____ **Date:**_____
Sampling Leader/Team:_____ **Laboratory Order Number(s):**_____

Project Sample Number	QC Duplicate Sample Number	QA Duplicate Sample Number	Lab Sent to	Date Collected	Matrix	Sample Type (QA/QC samples, trip blank, etc.)