CEDEN

California Environmental Data Exchange Network



Chemistry Data Submission Guidance Document

Updated October 20, 2022

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List of Acronyms

]]	California Environmental Data Exchange Network
LABQA	Laboratory Quality Assurance
RDC	Regional Data Center
SWAMP	Surface Water Ambient Monitoring Program
QAO	Quality Assurance Officer

List of Terms

Controlled Vocabulary	Controlled vocabulary refers to codes and associated definitions maintained within CEDEN to ensure comparability between and among data sets. Current controlled vocabulary contained within associated lookup lists can be found at: <u>http://ceden.org/CEDEN_checker/Checker/LookUpLists.php</u> . The process for adding new values can be found at: <u>http://ceden.org/vocabulary_request.shtml</u> .
Data Checker	Web-based automated tool that assists data submitters in examining their data sets against the required LookUp lists, formats and business rules.
LookUp Lists	Controlled vocabularies are maintained within the CEDEN database as "LookUp Lists" and are managed through individual RDCs to maintain comparability between RDCs and throughout data sets available through CEDEN.
Native Sample	Native sample refers to the environmental sample collected and analyzed. The native sample can be compared to field quality assurance samples (e.g. field duplicate, field blank) and laboratory quality assurance samples (e.g. laboratory duplicate, matrix spike).
Primary Key	Uniquely identifies each row in a table and is comprised of a set of columns. No two distinct rows in a table can have the same combination of column values. Required for record uniqueness.
Data Type	Refers to the type of format required for a specific column heading in CEDEN templates. Data type examples include: integer (whole numbers), text, date and time, and decimal.

Introduction

This document is designed to provide guidance on reporting requirements for electronic data to be entered in the California Environmental Data Exchange Network (CEDEN) templates. Detailed below are definitions of data elements and rules for formatting chemistry data within the CEDEN chemistry template. For information on entering laboratory QA samples and field generated QA samples see Appendix A. Please review the entire Chemistry Data Submission Guidance Document prior to filling out or submitting the CEDEN Chemistry Template. If you have any questions regarding these guidelines, you may contact the <u>CEDEN Help Desk</u> retain the services of one of the <u>Regional Data Center</u> (RDC) for help.

Regional Data Center	Contact	Phone	Email
(RDC)		Number	
Central Coast RDC	Stacey Swenson	831/771-4114	sswenson@mlml.calstate.edu
Central Valley RDC	Melissa Turner	530/756-5200	mturner@mlj-llc.com
San Francisco RDC	Cristina Grosso	510/746-7371	cristina@sfei.org

You may also contact the CEDEN Help Center at ceden@waterboards.ca.gov.

Chemistry Data Submission Steps

To submit water quality chemistry data to CEDEN, start with the CEDEN_Chemistry_Template Excel file, which can be found at: <u>http://ceden.org/ceden_datatemplates.shtml</u>. In this template you will find the three data tables (each in a separate worksheet) required for submitting chemistry data. This file can be named at the discretion of the user; however, the Excel sheet tabs **MUST** be named "**Locations**," "**ChemResults**" and "**LabBatch**," respectively.

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CEDEN Chemistry Template Tables

Below describes what is included and submission requirements for each of the 3 tables in the CEDEN Chemistry Template:

- 1. Locations
 - a. Holds information about location sampled
 - b. Required only if actual unique latitudes and longitudes were recorded for each sampling event.
- 2. ChemResults
 - a. Used to record chemistry analysis results
 - b. Required and must be submitted with LabBatch table
- 3. LabBatch
 - a. Used to record lab batch information necessary for analyzing the data
 - b. Required and must be submitted with ChemResults table.

The guidelines in the following sections will assist you in getting your data into the CEDEN Chemistry Template tables. However, if at any time you have questions more specific to your data, (e.g. adding new codes to LookUp lists) contact your local RDC.

Once you have placed your data into the CEDEN Chemistry Template tables, visit your RDC's website to check and submit your data. Regional Data Center information can be found at: <u>http://www.ceden.org/data_centers.shtml</u>. The online data submission process includes specific checks on your data to ensure both data integrity and comparability with other data sets. Once your data has passed all of the checks it will be uploaded into the centralized CEDEN database and become available through the CEDEN website (<u>www.ceden.org</u>).

Chemistry Template Data Tables

Locations Table

PURPOSE:

The locations table contains specific information about the locations sampled. Actual latitudes and longitudes are recorded here for each sampling event. In the event that only target latitudes and longitudes were recorded, it is sufficient to rely on the stations and associated details approved during the controlled vocabulary request process.

COLUMN REQUIREMENTS:

Columns within the CEDEN Chemistry Template tables are either considered 1) required, 2) desired or 3) not required. Required columns must be completed in order for data to be accepted by CEDEN. Desired columns are strongly encouraged and should be completed with known values, whenever possible. If the actual value is unknown, then the given default value **must** be used. Not required columns include additional information that aid in data usability. Individual column requirements are listed below:

Required Columns:

StationCode SampleDate ProjectCode CoordinateNumber ActualLatitude ActualLongitude Datum

Desired Columns:

EventCode ProtocolCode AgencyCode LocationCode CoordinateSource

Not Required Columns:

SampleComments GeometryShape Elevation UnitElevation StationDetailVerBy StationDetailVerDate StationDetailComments

LOCATIONS TABLE STRUCTURE:

CHEMISTRY TEMPLATE	DATA			LOOKUP	
HEADER	ТҮРЕ	REQUIRED	SIZE	LIST	DEFINITION
StationCode*	Text	Yes	25	Station LookUp	A code representing the StationName and site and should be unique within CEDEN. A single waterbody may have multiple stations. StationCodes and station information must be submitted to the CEDEN system via the new vocabulary request process before lab data can be submitted.
SampleDate*	Date/ Time	Yes	20		Refers to the date the sample was collected in the field; formatted as dd/mmm/yyyy.
ProjectCode*	Text	Yes	25	Project LookUp	References the project that is associated with the sample.
EventCode	Text	Desired	20	Event LookUp	Represents the primary reason (e.g. water quality, tissue or bioassessment sampling) of the sampling event at a particular station and date.
ProtocolCode	Text	Desired	50	Protocol LookUp	Represents the sampling protocol used, which includes the set of methods, methodology and/or specifications, such as "MPSL- DFG_Field_v1.0." Established protocols may be used or Regions may document their own sampling protocols. Use "Not Recorded" when environmental samples are taken using unknown protocols.
AgencyCode	Text	Desired	20	Agency LookUp	Refers to the organization or agency that collected the sample. This should be listed on the Chain of Custody (COC) document that accompanies the samples from the field. Use "Not Recorded" if unknown.
SampleComments	Text	No	255		Comments related to the GIS station information verification.
LocationCode	Text	Desired	50	Location LookUp	Describes the physical location in the waterbody where the sample was collected. One sampling event may have a single or multiple locations. Use "Not Recorded" if unknown.

* Primary Key, required for record uniqueness.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
GeometryShape	Text	No	50	Variable Codes LookUp; Geometry- ShapeList	Physical shape of the location. Example values are Line, Point, or Polygon.
CoordinateNumber	Integer	Yes			Number of coordinates recorded at a Location; e.g. 1 for Points (target and actual coordinates), 1 and 2 for Lines. Default value equals "1."
ActualLatitude	Decimal	Yes			Represents the actual latitude for the sample site in decimal degrees with 5 decimal places.
ActualLongitude	Decimal	Yes			Represents the actual longitude for the sample site in decimal degrees with 5 decimal places (must be negative).
Datum	Text	Yes	10	Variable Codes LookUp; DatumList	The Datum field records the datum that was used on the GPS Device to record the GPS measurements. Example = NAD83. If the datum is unknown, use "NR."
CoordinateSource	Text	Desired	50	Variable Codes LookUp; Coordinate- SourceList	Describes how the coordinate was measured. For example, if measurement was taken from a map or GPS. Use "NR" if unknown.
Elevation	Decimal	No			Elevation at which the sample was taken. Example = 1.
UnitElevation	Text	No	2	Variable Codes LookUp; Unit- Elevation- List	Unit of the Elevation measurement. Example = m
StationDetailVerBy	Text	No	100		Agency or person who performed the verification of the station detail information.
StationDetailVerDate	Date/ Time	No			Date the station detail information was verified; formatted as dd/mmm/yyyy.
StationDetailComments	Text	No	255		Comments related to the station detail information.

Chemistry Results Table

PURPOSE:

The purpose of the chemistry results table is to document the analysis results for water chemistry, bacteria and algae biomass. Note bacteria single species concentrations are stored within the following chemistry result table, whereas abundance bacteria are stored within the taxonomy template. Each record represents a result from a specific analysis for a single analyte in a single sample. This table will also contain all supporting QA sample results.

COLUMN REQUIREMENTS:

Columns within the CEDEN Chemistry Template tables are either considered 1) required, 2) desired or 3) not required. Required columns must be completed in order for data to be accepted by CEDEN. Desired columns are strongly encouraged and should be completed with known values, whenever possible. If the actual value is unknown, then the given default value **must** be used. Not required columns include additional information that aid in data usability. Individual column requirements are listed below:

Required Columns:

StationCode	UnitCollectionDepth	LabReplicate
SampleDate	LabBatch	Result
ProjectCode	AnalysisDate	ResQualCode
CollectionTime	MatrixName	MDL
CollectionMethodCode	MethodName	RL
SampleTypeCode	AnalyteName	QACode
Replicate	FractionName	-
CollectionDepth	UnitName	
S:		

Desired Columns

EventCode	ComplianceCode
ProtocolCode	DilutionFactor
AgencyCode	PrepPreservationName
LocationCode	PrepPreservationDate
CollectionDeviceName	DigestExtractMethod
PositionWaterColumn	DigestExtractDate

Not Required Columns:

SampleComments GeometryShape LabCollectionComments ExpectedValue SampleID LabSampleID LabResultComments

RESULTS TABLE STRUCTURE:

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
StationCode*	Text	Yes	25	Station LookUp	A code representing the StationName and site and should be unique within CEDEN. A single waterbody may have multiple stations. StationCodes and station information must be submitted to the CEDEN system via the new vocabulary request process before lab data can be submitted.
SampleDate*	Date/ Time	Yes			Refers to the date the sample was collected in the field. Formatted as dd/mmm/yyyy. Use "01/Jan/1950" if the actual SampleDate is unknown.
ProjectCode	Text	Yes	25	Project LookUp	References the project that is associated with the sample.
EventCode	Text	Desired	20	Event LookUp	Represents the primary reason (e.g. water quality, tissue or bioassessment sampling) of the sampling event at a particular station and date.
ProtocolCode	Text	Desired	50	Protocol LookUp	Represents the sampling protocol used, which includes the set of methods, methodology and/or specifications, such as "MPSL- DFG_Field_v1.0." Established protocols may be used or Regions may document their own sampling protocols. Use "Not Recorded" when environmental samples are taken using unknown protocols. Use "Not Applicable" when LabQA samples are taken with unknown protocols.
AgencyCode	Text	Desired	20	Agency LookUp	Refers to the organization or agency that collected the sample. This should be listed on the Chain of Custody (COC) document that accompanies the samples from the field. Use "Not Recorded" if unknown.
SampleComments	Text	No	255		The comments field should be used for any notes or comments specifically related to the sample collection.

* Primary Key, required for record uniqueness.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
LocationCode	Text	Desired	50	Location LookUp	Describes the physical location in the waterbody where the sample was collected. One sampling event may have a single or multiple locations. Use "Not Recorded" when environmental samples are taken at an unknown location. For LabQA samples utilize "Not Applicable."
GeometryShape	Text	No	50	Variable Codes LookUp; Geometry- ShapeList	Physical shape of the location. Example values are Line, Point, or Polygon.
CollectionTime*	Date/ Time	Yes	20		Refers to the time when the first sample of a sampling event at a specific station was collected in the field. Format equals hh:mm. Use "00:00" if the time sampling started is unknown.
CollectionMethodCode	Text	Yes	50	Collection Method LookUp	Refers to the general method of collection such as Sed_Grab, Sed_Core, Water_Grab, Autosampler24h, Autosampler7d. Use "Not Recorded" when environmental samples are taken using an unknown method. For LabQA samples utilize "Not Applicable."
SampleTypeCode*	Text	Yes	20	Sample Type LookUp	Refers to the type of sample collected or analyzed. Use "Not Recorded" if unknown.
Replicate*	Integer	Yes			Used to distinguish between replicates created at a single collection in the field. The default value is "1." Replicate samples are collected at the same station and date. Therefore, samples collected on different dates from the same station should both have a Replicate value of "1."
CollectionDeviceName	Text	Desired	50	Collection Device Lookup	Name of the CollectionDevice. Use "Not Recorded" if unknown.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
CollectionDepth	Decimal	Yes			Records the depth or penetration, from the surface in the water or sediment column, at which the sample was collected.
UnitCollectionDepth	Text	Yes	50	Variable Codes LookUp; Unit- Collection- DepthList	Refers to the units used in the CollectionDepth including cm (centimeters) and m (meters).
PositionWaterColumn	Text	Desired	20	Variable Codes LookUp; Position- Water- ColumnList	Position in water column where the sample was taken. Use "Not Applicable" if unknown.
LabCollectionComments	Text	No	255		Comments related to the LabCollection
LabBatch*	Text	Yes	35		The LabBatch is a unique code, provided by the laboratory, which represents a group of samples processed together. It groups all environmental samples with their supporting QC samples and will be used to verify completeness. This field is the primary key to ensure record uniqueness. To ensure uniqueness in the CEDEN system, the LabAgencyCode may be appended to this value when loaded to CEDEN. Please use a standard format to construct a composite Lab Batch. Format as LabBatch a dash (–) and the AgencyCode. Example: Batch1- SCCWRP. All LabBatch codes used on the ChemResults tab, must be detailed on the LabBatch tab.
AnalysisDate	Date/ Time	Yes			Date and time the sample was processed on the analytical instrument. Formatted as dd/mmm/yyyy hh:mm. Use "01/Jan/1950 00:00" if the actual date and time that the analysis was performed is unknown.
MatrixName*	Text	Yes	50	Matrix LookUp	Refers to the sample matrix, e.g. samplewater. Use "Not Recorded" if unknown.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
MethodName*	Text	Yes	50	Method LookUp	Refers to the analysis method used by the laboratory to analyze the sample. Use "Not Recorded" if the method used is unknown.
AnalyteName* Text		Yes	100	Analyte LookUp	Name of the analyte or parameter for which the analysis is conducted and result is reported. The LookUp list includes the acceptable abbreviation or name of the variable used by the database, enabling consistency across reporting.
FractionName*	Text	Yes	50Fraction LookUpSpecific descriptor example, metals a as total or dissolv this description s		Specific descriptor of the Analyte. For example, metals are often expressed as total or dissolved and therefore this description should be used within the fraction field.
		Refers to how the chemistry result is measured or expressed.			
LabReplicate*	Integer	Yes			Used to distinguish between replicates created in the laboratory. It differentiates the original field sample that was analyzed from all subsequent laboratory duplicates. The default is "1."
Result	Text	Yes	50		Final numeric result of a given analyte, stored as text to retain trailing zeros. The result should be reported with the appropriate number of significant figures. Result may be left blank as long as an appropriate ResQualCode is provided.
ResQualCode	Text	Yes	10	ResQual LookUp	Qualifies the analytical result of the sample. Use "=" if unknown.
MDL	Decimal	Yes			The MDL (method detection limit) is the lowest possible calculated detection limit associated with a given method and analyte. The MDL should be reported on the lab summary sheet with the associated measured result. If an MDL is not listed on the lab summary sheet, then the default value should be "-88" with a QACode of "NMDL."

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
RL	Decimal	Yes			The RL (reporting limit) of the sample analyzed is the minimum value below which data are documented as non-quantifiable, as determined by the laboratory. The default value of "-88" is utilized for analytes such as surrogates or grain size samples.
QACode*	Text	Yes	30	QA LookUp	Applied to the result to describe any special conditions, situations or outliers that occurred during or prior to the analysis to achieve the result. The default code, indicating no special conditions, is "None." Use "NR" if the special conditions are unknown or if it is unknown whether there were special conditions. If more than one code should be applied to a record, the convention is to list them in alphabetical order separated by commas and no spaces.
ComplianceCode	Text	Desired		Data Compliance LookUp	Unique code describing the compliance with the associated Quality Assurance Project Plan (QAPP). Use "NR" if the compliance is unknown.
DilutionFactor	Decimal	Desired			Factor by which a sample was diluted and is reported as a whole number. It is equal to the final volume divided by the initial volume of solution, or DF = Vf ÷ Vi. The default value is "1," meaning no dilution was performed.
ExpectedValue	Decimal	No			Concentration of the analyte in a reference standard, laboratory control sample or matrix spike sample or the value expected to be obtained from analysis of the QC Sample. This consists of the native sample result concentration plus the spike amount. For surrogate samples, the expected value should be 100, representing 100%.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
PrepPreservationName	Text	Desired	50	PrepPreser vation LookUp	References the preparation or preservation method performed on the samples prior to analysis. Use "Not Recorded" if the preparation or preservation method is unknown. Use "None" if no preparation or preservation was performed.
PrepPreservationDate	Date/ Time	Desired			Date and time the preparation or preservation was started. Use "01/Jan/1950 00:00" if the date and time the process started isn't known or if no process was performed.
DigestExtractMethod	Text	Desired	50	Digest Extract LookUp	References the digestion or extraction method performed on the sample prior to analysis. Use "Not Recorded" if the preparation or preservation method is unknown. Use "None" if no preparation or preservation was performed.
DigestExtractDate	Date/ Time	Desired			Date and time the digestion or extraction was started. Use "01/Jan/1950 00:00" if the date and time the process started isn't known or if no process was performed.
SampleID	Text	No	40		Unique identifier supplied by the organization directing the sampling or sampling agency and is used to track the sample throughout the sampling and analysis processes. This field can be used to tie a result to the sample.
LabSampleID	Text	No	35		Recommended field intended to provide lab specific identification for an analyzed sample.
LabResultComments	Text	No	130		Holds any comments related to the lab result or analysis of the sample.

Chemistry LabBatch Table

PURPOSE:

The chemistry LabBatch table contains information about lab batches. A batch represents a group of samples processed together. It groups all environmental samples with their supporting QA samples. Review method or project specific requirements for specific batch definitions. Each project or method might have different requirements for a batch. An example batch for methods with no digestions or extractions would include all samples (including QA samples) processed by a single lab, within a 24 hour period, using a single preparation and analytical method. An example batch for methods with digestions or extractions would include all samples or extractions would include all samples processed by a single lab, digested or extracted together, using a single preparation and analytical method. In some cases, a batch may include analyses for several analytes (as with most metals); in other cases, only a single analyte is included within a batch (as with Hardness as CaCO3). If your project requires QA samples, these are expected to be submitted with each batch

COLUMN REQUIREMENTS:

Columns within the CEDEN Chemistry Template tables are either considered 1) required, 2) desired or 3) not required. Required columns must be completed in order for data to be accepted by CEDEN. Desired columns are strongly encouraged and should be completed with known values, whenever possible. If the actual value is unknown, then the given default value **must** be used. Not required columns include additional information that aid in data usability. Individual column requirements are listed below:

Required Columns:

LabBatch LabAgencyCode

Desired Columns:

LabSubmissionCode BatchVerificationCode

Not Required Columns:

SubmittingAgencyCode LabBatchComments

LABBATCH TABLE STRUCTURE:

* Primary Key, required for record uniqueness.

* Primary Key, required for		quenessi		LOOVUD	
CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
LabBatch*	Text	Yes	35		The LabBatch is a unique code, provided by the laboratory, which represents a group of samples processed together. It groups all environmental samples with their supporting QC samples and will be used to verify completeness. This field is the primary key to ensure record uniqueness. To ensure uniqueness in the CEDEN system, the LabAgencyCode may be appended to this value when loaded to CEDEN. Please use a standard format to construct a composite Lab Batch. Format as LabBatch a dash – and the AgencyCode. Example: Batch1- SCCWRP. All LabBatch codes used on the ChemResults tab must be detailed on the LabBatch tab.
LabAgencyCode*	Text	Yes	20	Agency LookUp	LabAgencyCode refers to the organization, agency or laboratory that performed the analysis on the sample. Use "Not Recorded" if the agency is unknown.
LabSubmissionCode	Text	Desired	10	Lab Submission Lookup	The LabSubmissionCode is a unique batch qualifier code assigned to the LabBatch as a whole that references the quality of the data in the LabBatch. The LabSubmissionCode is assigned by the analyzing laboratory, but should be reviewed by the Project Manager or other appropriate person to ensure that the code has been applied based on project specific data quality objectives and criteria. Use "NR" if the code is unknown.
BatchVerificationCode	Text	Desired	10	Batch Verification Lookup	Unique code referencing the Verification of a Batch. Use "NR" if unknown.
SubmittingAgencyCode	Text	No	20	Agency LookUp	Organization or agency that is responsible for submission of the data to the database. This agency may be different from LabAgencyCode if the analytical data were subcontracted to another agency.

CHEMISTRY TEMPLATE HEADER	DATA TYPE	REQUIRED	SIZE	LOOKUP LIST	DEFINITION
LabBatchComments	Text	No	255		LabBatchComments records any comments relating to the LabBatch as a whole. Comments should explain any irregularities in sample processing.

Appendix A: Specific Entry for Laboratory and Field Generated QA Samples

INTRODUCTION

Appendix A has been created to give additional guidance regarding business rules and formatting of quality assurance data generated in the laboratory or in the field. The following sections on Laboratory QA Samples and Field Generated QA Samples list example values that can be used to ensure comparability with other QA samples generated with different projects. The example values are listed for a subset of the Chemistry Template columns and are associated with descriptions and business rules to further guide the data generator in how to format quality assurance data. The examples only reference a subset of the columns in the Chemistry Template; the Chemistry Data Submission Guidance Document main body should be used as a reference for definitions and associated lookup lists for how to populate the additional columns not addressed in the examples.

1. LABORATORY QA SAMPLES

The sections below provide examples for entering the following types of data into the chemistry templates:

- 1.1. Samples that are generated or created by a laboratory (LABQA)
- 1.2. Environmental samples that are modified by a laboratory for QA purposes (e.g. matrix spikes)

1.1 LABORATORY GENERATED QA SAMPLES (LABQA)

All samples generated from within the laboratory, such as a lab blank, laboratory control spike (LCS), or certified reference material (CRM), are entered into the chemistry template according to specific business rules. Table 1 is an example of the values that should be entered for laboratory generated QA (LABQA) samples within the chemistry template columns. Descriptions are included in Table 1 (Description & Business Rules) to further address formatting specifications, give additional details and note business rules. Specific business rules may vary by project and RDC; please check with your RDC to ensure appropriate business rules are being followed and/or any changes are appropriately documented.

Table 1. Example values to be used for laboratory generated QA samples (LABQA) for a subset of chemistry template columns.

Chemistry Template Header	Value	Description & Business Rules
StationCode	LABQA	"LABQA" is used as the station code for any sample generated in the laboratory including lab blanks, LCS and CRMs.
SampleDate		The SampleDate of a LABQA samples reflects the date that the sample was created within the laboratory. SampleDate must be equal to or before AnalysisDate and expressed as dd/mmm/yyyy.
ProjectCode		Populate with the associated project code within Project LookUp or use default value of "Not Applicable."

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Chemistry Template Header	Value	Description & Business Rules
EventCode	WQ	For water and sediment chemistry use "WQ." See the EventCode LookUp list for additional EventCodes and associated definitions. The EventCode should be consistent with the environmental samples in the same batch.
ProtocolCode		Populate with applicable ProtocolCode within Protocol LookUp or use default value of "Not Applicable."
AgencyCode		Organization or agency that analyzed the sample. Select from Agency LookUp list or utilize the null value of "Not Recorded."
LocationCode	Not Applicable	LABQA samples are generated in the laboratory and therefore are associated with a LocationCode of "Not Applicable."
GeometryShape		Leave blank
		LABQA are associated with 00:00 time for collection since they are generated in the laboratory.
CollectionTime	00:00	BR: There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different CollectionTime. For example, when more than one CNEG is analyzed in the same batch but are not replicates of each other, one CollectionTime should be 0:00 and the other 0:15, increasing the time by 15 minutes for each additional sample. Adjusting the Replicate to differentiate between samples is also acceptable.
CollectionMethodCode	Not Applicable	LABQA samples are generated in the laboratory and therefore are not associated with a sample LocationCode.
SampleTypeCode	LabBlank, LCS or CRM	Select from SampleTypeLookUp List – LabBlank, LCS and CRM are listed as the most common LABQA sample types.
Replicate	1	BR: There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different CollectionTime (See collection time for details) or Replicate.
CollectionDeviceName		Leave blank; there is no CollectionDeviceName associated with LABQA and this field does not need to be populated.
CollectionDepth	-88	"-88" is used as a null value for LABQA samples. This field must be populated with a number and cannot be left blank.
UnitCollectionDepth	 cm	For water use "m" for meter. For sediment use "cm" for centimeter.
PositionWaterColumn	Not Applicable	LABQA samples are generated in the laboratory and therefore there is associated with the PositionWaterColumn value of "Not Applicable."
	labwater	See Matrix LookUp for definition.
Martan	blankwater	See Matrix LookUp for definition.
Matrix	blankmatrix	See Matrix LookUp for definition.
	sediment	See Matrix LookUp for definition.
LabReplicate	1 2	Use a LabReplicate of "1" for the original LABQA sample. Use a LabReplicate of "2" for a duplicate LABQA sample.

BR: Business Rule

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1.2 LABORATORY MODIFIED QA SAMPLES

There are several types of samples discussed in this section that are generated or modified within the laboratory. The first is a matrix spike, which is a modified, or analyte-spiked, field sample. The second is a laboratory generated duplicate of a field sample. At times, laboratories use samples not generated through the data generator's project to satisfy project specific batch QA requirements. This third type is a non-project sample.

1.2.1 MATRIX SPIKE AND LABORATORY DUPLICATE SAMPLES

For matrix spike samples (collected by the project) and laboratory duplicate samples performed on project sample (native field sample), all fields describing the sample (StationCode, EventCode, ProtocolCode, LocationCode, SampleDate, CollectionTime, CollectionMethodCode, CollectionDepth, UnitCollectionDepth, ProjectCode, AgencyCode) remain the same as the native sample. For matrix spike samples, the only fields that are different than the native field sample are SampleTypeCode and potentially the Replicate. For laboratory generated duplicate samples, the only field that is different than the native field sample is the LabReplicate. Table 2 lists the column headers in the chemistry template that describe the sample and give example values and associated descriptions/business rules to aid the data generator in populating those fields for their own data.

Chemistry Template Header	Value	Description & Business Rules	
StationCode		Same as native field sample	
SampleDate		Same as native field sample	
ProjectCode		Same as native field sample	
EventCode		Same as native field sample	
ProtocolCode		Same as native field sample	
AgencyCode		Same as native field sample	
LocationCode		Same as native field sample	
GeometryShape		Same as native field sample	
CollectionTime		Same as native field sample	
CollectionMethodCode		Same as native field sample	
		For laboratory generated duplicates this is the same SampleTypeCode as the native field sample.	
	MS1	Matrix Spike performed on a Grab or Integrated sample	
SampleTypeCode	MS2	Matrix Spike performed on a field duplicate sample (native field sample will have a SampleTypeCode of Grab or Integrated with a Replicate of 2).	
	MSBLDup	Matrix Spike performed on a field blind duplicate (FieldBLDup).	

Table 2. Example values to be used for matrix spike and laboratory duplicate samples created from project specific samples (native field sample).

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Chemistry Template Header	Value	Description & Business Rules
		BR: There are situations when a Matrix Spike was unintentionally performed on a blank sample such as a FieldBlank, TravelBlank, EquipBlank, DIBlank or FilterBlank. A batch may include two or more of these types of native samples where the only difference between them is the environmental sample's SampleTypeCode. The only way to differentiate between them is to give each a different CollectionTime. For example, when a batch contains both a DIBlank and an EquipBlank (both with an original time of 0:00) and a Matrix Spike was performed on the EquipBlank, one CollectionTime should be 0:00 and the other 0:15. Then the associated native sample CollectionTime should correspond to the MS1 sample times. For example, the EquipBlank would have a native sample time of 00:00 and an MS1 time of 00:00 and the DIBlank would have a native sample time of 00:15 (updated from 00:00).
Replicate	1	
CollectionDeviceName		Same as native field sample
CollectionDepth		Same as native field sample
UnitCollectionDepth		Same as native field sample
Matrix		Same as native field sample
LabDaulianta	1	Native field sample or Matrix Spike
LabReplicate	2	Laboratory generated duplicate or Matrix Spike duplicate

BR = Business Rule

1.2.1.1 Matrix Spike Samples performed on Field Duplicates

Table 3 describes the way to format matrix spike samples performed on field duplicates (Replicate = 2), field blind duplicates (FieldBLDup), and composite blind duplicates (CompBLDup) in CEDEN as well as coding duplicate samples.

Table 3. Formatting field duplicates and matrix spikes.

	Chemistry	Template	Header	
	Sample Type		Lab	
Descriptions	Code	Replicate	Replicate	
1 One environmental sample: sampled or split in triplicate				
Single environmental sample	Grab	1	1	
Field duplicate of single environmental sample	Grab	2	1	
Second field duplicate of single environmental sample	Grab	3	1	
One environmental sample: sampled or split in triplicate submitted to the laboratory blind (unknown to the	and			
2 laboratory)				
Single environmental sample	Grab	1	1	

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		Chemistry	Template	Header
		Sample Type		Lab
	Descriptions	Code	Replicate	Replicate
	^ 	FieldBLDup or	-	•
	Field blind duplicate of single environmental sample	CompBLDup	1	1
		FieldBLDup or		
	Second field blind duplicate of single environmental sample	CompBLDup	2	1
3	One pair of MS/MSD: associated to one grab		•	
	Single environmental sample	Grab	1	1
	Matrix spike of single environmental sample	MS1	1	1
	Matrix spike duplicate of single environmental sample	MS1	1	2
			_	
<u> </u>	One pair of MS/MSD: associated to one grab with field	1	1	
4	duplicate present			
	Single environmental sample	Grab	1	1
	Field duplicate of single environmental sample	Grab	2	1
	Matrix spike of single environmental sample	MS1	1	1
	Matrix spike duplicate of single environmental sample	MS1	1	2
		1401	1	
5	One pair of MS/MSD: associated to one field duplicate			
	Single environmental sample	Grab	1	1
	Field duplicate of single environmental sample	Grab	2	1
	Matrix spike of field duplicate sample	MS2	1	1
	Matrix spike duplicate of field duplicate sample	MS2	1	2
		14132	1	L
6	One pair of MS/MSD: associated to one field blind duplicate		l	
0	Single environmental sample	Grab	1	1
		FieldBLDup or		1
	Field blind duplicate of single environmental sample	CompBLDup	1	1
	Matrix spike of field blind duplicate sample	MSBLDup	1	1
	Matrix spike duplicate of field blind duplicate sample	MSBLDup	1	2
		Mobilbup		
	Two pairs of MS/MSD: one associated to the grab and one			
7	associated to the field duplicate			
<u> </u>	Single environmental sample	Grab	1	1
-	Field duplicate of single environmental sample	Grab	2	1
<u> </u>	Matrix spike of single environmental sample	MS1	1	1
	Matrix spike of single environmental sample	MS1 MS1	1	2
	Matrix spike dupicate of single environmental sample	MS1 MS2	1	1
	Matrix spike duplicate of field duplicate sample	MS2 MS2	1	2
L	practic spike auplicate of held auplicate sample	14132	1	4

1.2.2 NON-PROJECT MATRIX SPIKE AND DUPLICATE SAMPLES (000NONPJ)

At times, laboratories use samples not generated through the project to satisfy batch QA requirements. These samples have different formatting rules, which are displayed in Table 4. In most cases, non-project samples have no sample collection information since they are used only to satisfy batch QA requirements. Please contact your RDC if the formatting rules in Table 4 are not applicable to non-project data for your data set.

Chemistry Template Header	Value	Description & Business Rules
StationCode	000NONPJ	"000NONPJ" is the StationCode associated with an environmental sample that was collected by a different project but used for laboratory quality assurance purposes (i.e. duplicate or matrix spike).
SampleDate		SampleDate must be equal to or before AnalysisDate and expressed as dd/mmm/yyyy. Suggested date would be the earliest date of manipulation.
ProjectCode		Utilize ProjectCode of 000NONPJ sample or default value of "Not Applicable" if not known.
EventCode	WQ	For water and sediment chemistry use "WQ". See the EventCode LookUp list for additional EventCodes and associated definitions. The EventCode should be consistent with the environmental samples in the same batch.
ProtocolCode		Utilize ProtocolCode of 000NONPJ sample or default value of "Not Applicable" if not known.
AgencyCode		Organization or agency that analyzed the sample. Select from Agency LookUp list. Use "Not Recorded" if unknown.
LocationCode		Utilize LocationCode of 000NONPJ sample or null value of "Not Recorded" if not known.
Geometry Shape		Leave blank.
CollectionTime		Utilize CollectionTime of 000NONPJ sample or null value of 00:00 if not known. BR: There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different CollectionTime. For example, when more than one LabBlank, CRM, or LCS is digested, extracted, or analyzed in the same batch on the same day but are not replicates of each other, one CollectionTime should be 0:00 and the other 0:15, increasing the time by 15 minutes for each additional sample. Adjusting the Replicate to differentiate between samples is also acceptable.
CollectionMethodCode		Utilize CollectionMethodCode of 000NONPJ sample or null value of "Not Recorded" if not known.

Table 4. Example values to be used with non-project (000NONPJ) matrix spike and duplicates samples and associated business rules.

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Chemistry Template Header	Value	Description & Business Rules		
		Select from the SampleTypeCode LookUp list for 000NONPJ laboratory duplicates. Use "Not Recorded" if SampleType is unknown.		
SampleTypeCode	MS1	"MS1" is used for laboratory matrix spikes created with 000NONPJ samples. See <i>Table 3: Formatting field duplicated and</i> <i>matrix spikes</i> for additional business rules regarding matrix spikes.		
		Utilize Replicate of 000NONPJ sample or default value of "1" if not known.		
Replicate		BR: There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different CollectionTime (See <i>CollectionTime</i> for details) or Replicate.		
CollectionDeviceName		Utilize CollectionDeviceName of 000NONPJ sample or leave blank if not known.		
CollectionDepth		Utilize CollectionDepth of 000NONPJ sample or null value of "- 88" if not known. This field must be populated with a number and cannot be left blank.		
UnitCollectionDepth	_m cm	For water use "m" for meter. For sediment use "cm" for centimeter.		
PositionWaterColumn		Utilize PositionWaterColumn of 000NONPJ sample or default value of "Not Applicable."		
Matrix		Utilize Matrix of 000NONPJ sample. If the actual matrix is not known, use "samplewater" for water samples and "sediment" for sediment samples.		
	QAX	"QAX" is associated with 000NONPJ samples when the native sample is not included in the batch reported.		
QACode	None	If the batch includes the native 000NONPJ sample result as well as the laboratory quality assurance 000NONPJ sample, "None" or appropriate QACode to indicate recoveries outside criteria or other QA issues (see QACode Lookup list).		
Preparation Preservation		Actual preparation or preservation performed. This should be the same as the other samples in the batch.		
Preparation Preservation Date		Actual preparation or preservation date and time expressed as dd/mmm/yyyy hh:mm		
LabReplicate	1	Original 000NONPJ samples and original 000NONPJ matrix spike samples are associated with a LabReplicate of "1".		
L.	2	Matrix spike duplicates and laboratory duplicates are associated with a LabReplicate of "2".		
SampleID		The <i>LabSampleID</i> or <i>Source ID</i> can be used here as the <i>SampleID</i> as an indicator to identify the native sample. This column may be left blank.		
LabSampleID		Recommended - provide lab specific identification for an analyzed sample. It is preferable to add -Dup, -MS, -MSD to the end of the Lab ID to help confirm the SampleTypeCode and the LabSampleID of the native sample. This column can be left blank.		

BR = Business Rule

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There are two types of blank samples discussed in this section that are generated as field quality assurance samples. The first is when a field generated QA sample is created at a specific station and that station information is important to record. For example, some projects may allow a certain amount to be detected in the blank provided it is less than five times the native (environmental) sample. For those situations it would be important to have similar sample information between the blank and the native sample to evaluate quality assurance criteria. The second example is when a field generated QA sample is created for a sampling trip or if the station information is not recorded.

Field duplicate samples should be associated with a station and that information should be the same as the native sample such that the sample collection information is identical between the field duplicate and native sample except that the field duplicate is associated with a Replicate of "2." Therefore, the following section is specific to field generated blanks.

2.1 FIELD GENERATED BLANK SAMPLES – STATION SPECIFIC

For analyses that require an EquipBlank, TravelBlank, FieldBlank, or FilterBlank to accompany a sampling event and where it is important to record the station information, the data are entered into CEDEN in the same manner as the native samples collected at that station. Table 5 lists the chemistry template column headers and associated descriptions and business rules for guidance.

Table 5. Example values to be used for field generated blank samples associated with station specific details.

Chemistry Template Header	Value	Description & Business Rules		
StationCode		Same as native sample. BR: For EquipBlanks, TravelBlanks or FilterBlanks that may be created at a laboratory or agency prior to sampling, a StationCode may still be applied to the sample if it serves the purpose of the project to associate all field and laboratory QA samples together (i.e. via the same sample entry information).		
SampleDate		Same as native sample.		
ProjectCode		Same as native sample.		
EventCode	WQ	Same as native sample. For water and sediment chemistry use "WQ."		
ProtocolCode		Same as native sample.		
AgencyCode		Same as native sample.		
LocationCode		Same as native sample.		
GeometryShape		Same as native sample.		
CollectionTime		Time sample was created (same as native sample time) or "00:00." There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different <i>CollectionTime</i> . For example, when more than one EquipBlank, FieldBlank, or FilterBlank is created on the same day but are not replicates of each other, one <i>CollectionTime</i> should be 00:00 and the other 00:15, increasing the time by 15 minutes for each additional sample.		
CollectionMethodCode	Not Applicable	Field generated blanks are associated with the CollectionMethodCode of "Not Applicable."		
SampleTypeCode	EquipBlank, TravelBlank, FieldBlank or FilterBlank	See the SampleTypeCode LookUp list for definitions of the various field generated QA SampleTypeCodes.		
Replicate	1	Field generated blanks should have a replicate of "1."		
CollectionDeviceName	Not Applicable	Field generated blanks are associated with the CollectionDeviceName of "Not Applicable."		
CollectionDepth	-88	Field generated blanks are not generated using environmental water and therefore are associated with a null value (-88) for CollectionDepth.		
UnitCollectionDepth	m	For water use "m" for meter.		
LabCollection Comments		It is recommended that when an equipment blank (EquipBlank) is generated, a comment is recorded that lists the type of equipment cleaned and location (lab or field). A value is not required for this field and can be left blank.		
Matrix	Labwater or blankwater	See Matrix LookUp for definitions.		
LabSampleID		Recommended - provide lab specific identification for an analyzed sample.		

BR = Business Rule

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Appendix A – Specific Entry for Laboratory and Field Generated QA Samples

2.2 FIELD GENERATED BLANK SAMPLES (FIELDQA) – NON STATION SPECIFIC

For analyses that require an EquipBlank, FieldBlank, FilterBlank, TravelBlank or DIBlank to accompany a sampling event and it is not important to record the station information, the data are not associated with specific sample collection information. Table 6 lists example values that are to be used for generic blank samples generated in the field and associated description and business rules that can be used for guidance for data entry.

Table 6. Example of values to be used for field generated blank samples that are not associated with station specific details (FIELDQA).

Chemistry Template Header	Value	Description & Business Rules		
StationCode	FIELDQA	Field generated blanks not associated with a specific station are associated with the StationCode "FIELDQA."		
SampleDate		Date that the sample was created. BR: TravelBlank should be entered as the date the TravelBlank becomes part of the sample group (i.e., leaves the lab for the sampling event).		
ProjectCode		Project associated with the sample.		
EventCode	WQ	Same as native sample. For water and sediment chemistry use "WQ."		
ProtocolCode		Protocol used or "Not Recorded."		
AgencyCode		Organization or agency that created the sample.		
LocationCode	Not Applicable	Since the FIELDQA blank sample is not associated with a specific station, the LocationCode is "Not Applicable."		
GeometryShape	Not Applicable	Since the FIELDQA blank sample is not associated with a specific station, the GeometryShape is "Not Applicable."		
CollectionTime		Time sample was created or "00:00." There are situations within a batch when two identical sample types are used for QA reasons and the only way to differentiate between them is to give them each a different <i>CollectionTime</i> . For example, when more than one EquipBlank, FieldBlank, or FilterBlank is created on the same day but are not replicates of each other, one <i>CollectionTime</i> should be 00:00 and the other 00:15, increasing the time by 15 minutes for each additional sample.		
CollectionMethodCode	Not Applicable	Field generated blanks including FIELDQA are associated with the CollectionMethodCode of "Not Applicable."		
SampleTypeCode	EquipBlank, TravelBlank, FieldBlank, FilterBlank or DIBlank	See the SampleTypeCode lookup list for definitions of the various field generated QA SampleTypeCodes.		
Replicate	1	Field generated blanks including FIELDQA should have a replicate of "1."		

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Chemistry Template Header	Value	Description & Business Rules	
CollectionDeviceName	Not Applicable Field generated blanks including FIELDQA are associated with the CollectionDeviceName of "Not Applicable."		
CollectionDepth	-88	Field generated blanks including FIELDQA are not generated using environmental water and therefore are associated with a null value (-88) for CollectionDepth.	
UnitCollectionDepth	m	For water use "m" for meter.	
LabCollection Comments		It is recommended that when an equipment blank (EquipBlank) is generated, a comment is recorded that lists the type of equipment cleaned and location (lab or field).A value is not required for this field and can be left blank.	
Matrix	Labwater or blankwater	See MatrixLookup for definitions.	
LabSampleID		Recommended - provide lab specific identification for an analyzed sample.	

BR = Business Rule

Appendix B: Chemistry Data Submission Guidance Documentation Amendments

Amendments

Amendments made to the CEDEN Chemistry Data Submission Guidance Document are documented within Table 1.

Date of Amendment	Document Section	Amendment Summary	Amendment Details
August 23rd 2013	List of Acronyms	Added acronyms.	Added SWAMP and QAO to the List of Acronyms.
August 23rd 2013	Stations Table: Column Requirements	Updated required field designations for Stations Table.	Updated required field designations for Stations Table. Required Columns: Added: StationAgency, SWRCBWatTypeCode. Desired Columns: Added: CoordinateSource Removed: LocalWatershed, LocalWaterbody, Counties_2004_County, SWRCBWatTypeCode, CalWater_2004_RB. Not Required Columns: Added:EventType1, EventType2, EventType3, LocalWaterShed, LocalWaterBody, Counties_2004_COUNTY, CalWater_2004_RB, NHD_PlusCatchmentComID. Removed: CalWater_2004_SWRCBNUM2 HydrologicUnit
August 23rd 2013	Stations Table	Added Additional Resources section to Stations Table.	Added an "Additional Resources" section to the Stations Table after Column Requirements.
August 23rd 2013	Stations Table: Stations Table Structure: StationSource	Updated StationSource LookUp list and definition.	Updated StationSource LookUp List from blank to "AgencyLookUp or ProjectLookUp".Updated Definition from "Agency or project that created the station." to "Agency or project that submitted the station to CEDEN".
August 23rd 2013	Stations Table: Stations Table Structure	Added new fields to the Stations Table.	Added new fields to Stations Table Structure: StationAgency, EventType1, EventType2, EventType3 and NHD_Plus_CatchmentComID.

Date of Amendment	Document Section	Amendment Summary	Amendment Details
August 23rd 2013	Stations Table: Stations Table Structure: AddDate	Added format information to AddDate	Added "Format as dd/mmm/yyyy" to the AddDate definition.
August 23rd 2013	Stations Table: Stations Table Structure	Added default value information to Stations Table definitions.	Added default value information to the description field within the Stations Table for CoordinateNumber, Datum, CoordinateSource, SWRCBWatTypeCode
August 23rd 2013	Stations Table: Stations Table Structure: State	Added LookUp list information to State.	Updated State LookUp List from blank to "VariableCodesLookUp".
August 23rd 2013	Stations Table: Stations Table Structure	Updated Stations Table template header names.	Updated Stations Table template header names: "NHD24K_GNIS_Name" to "NHD_24K_v2_GNIS_Name", "NHD24k_Reachcode" to "NHD_24k_v2_ReachCode", "NHD24k_HUC12" to "NHD_24k_v2_HUC_12" and "NHD24k_Hu_12_Name" to "NHD_24k_v2_Name".
August 23rd 2013	Chemistry LabBatch Table: Column Requirements	Updated required field designations for Chemistry LabBatch Table.	Updated required field designations for Chemistry LabBatch Table: Required Columns: Added: LabAgencyCode. Desired Columns: Removed: LabAgencyCode,
August 23rd 2013	Chemistry LabBatch Table: LabBatch Table Structure	Added default value information to LabBatch Table definitions.	Added default value information to the description field within the LabAgencyCode, LabSubmissionCode and BatchVerificationCode.
August 23rd 2013	Chemistry Results Table: Purpose	Updated the Chemistry Results Table purpose section to specify where bacteria results are stored within CEDEN.	Updated Chemistry Results Table purpose language from "The purpose of the chemistry results table is to document the analysis results for water chemistry and algae biomass. Each record represents a result from a specific analysis for a single analyte in a single sample. This table will also contain all supporting QA sample results" to "The purpose of the chemistry results table is to document the analysis results for water chemistry, bacteria and algae biomass. Note bacteria single species concentrations are stored within the following chemistry result table, whereas abundance bacteria are stored within the taxonomy template. Each record represents a result from a specific analysis for a single analyte in a single sample. This table will also contain all supporting QA sample results."

Date of Amendment	Document Section	Amendment Summary	Amendment Details
August 23rd 2013	Chemistry Results Table: Column Requirements	Updated required field designations for Chemistry Results Table.	Updated required field designations for Chemistry Results Table: Desired Columns: Added: EventCode, PositionWaterColumn; Removed: ExpectedValue. Not Required Columns: Added: ExpectedValue; Removed: PositionWaterColumn,
August 23rd 2013	Chemistry Results Table: Stations Table Structure	Added default value information to Results Table definitions.	Added default value information to the description field within the SampleDate, ProtocolCode, AgencyCode, LocationCode, CollectionTime, CollectionMethodCode, SampleTypeCode, CollectionDeviceName, PositionWaterColumn, AnalysisDate, MatrixName, MethodName, ResQualCode, QACode, ComplianceCode, PrepPreservationName, PrePreservationDate, DigestExtractMethod, and DigestExtractDate.
August 23rd 2013	Chemistry Results Table: Stations Table Structure: Result	Added language to Result definition.	Added the following language to the Results field: "Result may be left blank as long as an appropriate ResQualCode is provided."
August 23rd 2013	Chemistry Results Table: Stations Table Structure: DilutionFactor	Updated Data Type for DilutionFactor	Updated DilutionFactor Data Type from Integer to Decimal.
October 11 th 2013	Introduction	Updated Southern California RDC contact information.	Updated Southern California RDC contact information from Shelly Moore to Marlene Hanken contact information.
March 17 th 2014	Appendix A	Updated Table 1 Matrix Descriptions	Updated Table 1 Matrix descriptions to "See Matrix LookUp for definition."
January 3 rd , 2017	Introduction, Station Table, and Chemistry Table	Removed references to Stations tab	Removed the Stations section and references to Stations tab, updated effected screen shot, and modified StationCode definition to note that station codes must be established through the new vocabulary request process prior to subittal.

Date of Amendment	Document Section	Amendment Summary	Amendment Details
January 3 rd , 2017	All	Updated use of quotes	Replaced single quotes with double quotes.
January 3 rd , 2017	Locations Table, Chemistry Results Table, LabBatch Table	Updated description of "desired" fields	Added reference to using default values when actual values are not know for "desired" fields in the "Column Requirements" paragraph.
January 3 rd , 2017	List of Terms	Updated links	Added current links for the LookUp lists and vocabulary request process.
January 3 rd , 2017	Introduction	Updated Central Coast RDC contact information	Updated the Central Coast RDC contact information from Mark Pranger to Stacey Swenson.
January 3 rd , 2017	Chemistry Table and LabBatch Table	Switched order of sections	Moved Chemistry Table to be before LabBatch table to reflect the order in the template.
January 3 rd , 2017	Locations Table, Chemistry Results Table, LabBatch Table	Modified use of "default" wording	Changed most instances of "Default equalsif unknown" to "Useif unknown."
January 3 rd , 2017	All	Various edits	Removed double spaces and duplicate words and other small edits.
January 3 rd , 2017	Locations Table and Chemistry Results Table	Updated StationCode definition	Included that StationCode must be unique within CEDEN, not just within the study design, as previously stated.
January 8 th , 2019	Introduction	Updated RDCs	Removed SCCWRP as current RDC.
January 8 th , 2019	Locations Table, Chemistry Results Table, LabBatch Table	Updated wording for "desired" (default required) fields	Changed "should" to "must" for "desired" fields in the "Column Requirements" paragraphs.
January 8 th , 2019	Locations Table and Chemistry Results Table	Variable Code List references	Added references to the appropriate lists in the Lookup List columns for fields that rely on Variable Codes.
October 20 th , 2022	Appendix C	Added Appendix C	Added Appendix C: Isotope Dilution Analyses Business Rules.
October 20 th , 2022	Appendix D	Added Appendix D	Added Appendix D: Passive Sampler Data Entry Guidance.
October 20 th , 2022	Introduction	CEDEN Help Desk	Added reference to contacting the CEDEN Help Desk with link to email.

Appendix C: Isotope Dilution Analyses Business Rules

CEDEN Business Rules: Isotope Dilution Analyses

This document provides business rules for recording analytical results in CEDEN derived from methods that use isotope dilution analysis (Isotope Dilution methods). Isotope dilution methods use signal ratios of added isotopically-labelled analyte (isotope dilution analogues) to unknown target analyte to measure analyte concentrations.

Naming Conventions for Isotope Dilution Analogues

The proposed naming conventions are similar to those for surrogates. The isotopically-labelled analyte name shall include the parenthetical abbreviation for isotope dilution analogue: (IsoDilAnalogue). The description shall include the phrase "Isotope Dilution Analogue" with a colon at the beginning of the description.

Example:

Analyte Name: Perfluorooctanesulfonic acid-13C8 (IsoDilAnalogue) Analyte Description: Isotope Dilution Analogue: Perfluorooctanesulfonic acid-13C8

Results Entry

- For analytes quantified via a signal ratio to an Isotope Dilution Analogue, add the QA Code of IDA
- For analytes that were not quantified using a signal ratio to an Isotope Dilution Analogue but were analyzed via an Isotope Dilution Method, no QA Code is needed to indicate that it was quantified using the calibration curve
- Isotope Dilution Analogue results must be reported with units of % recovery.
- If the isotopically-labelled analyte is used as a traditional internal standard (not correcting target analyte results), then the internal standard results should not be reported. Only the % recovery results of the IDA should be reported.
- Use the QA Code GIDA when the recovery was not within control limits on both the Isotope Dilution Analogue and the target analyte(s) that were quantified with that IDA.

OA	Code

QA Code	QA Name
IDA	Isotope Dilution Analogue corrected
GIDA	Isotope Dilution Analogue recovery not within control limits

Appendix D: Passive Sampler Data Entry Guidance

Passive Sampler-Related Entry

Passive Samplers consist of sorbent contained within a housing canister. They do not have moving parts¹ and can be left in the waterbody to be sampled from a couple of days to several weeks, resulting in an indication of analyte within the waterbody over time. The results of sorbent analysis provide a mass of analyte per sampler², not the typical mass per volume of sample water. For some types of passive samplers, the analyte mass per sample volume of water can be calculated, though the equations and coefficients change depending on the analyte of interest, device and sorbent used, and environmental conditions present during deployment. In some cases, the coefficients may not be known, or the model being used not well understood so deriving an accurate sample water concentration may be difficult. Therefore, the priority is to enter the results of the sorbent analysis, and use the metadata specified below to inform the data user that the results are not comparable to most of the other data in CEDEN. However, Semi-permeable Membrane Device (SPMD) passive samplers are well understood and the coefficients documented. For these results the data provider shall add the calculated aqueous concentration.

These business rules are meant to provide guidance on entering passive sampler monitoring results in the CEDEN Chemistry results template and to aid in user interpretation. Not all template columns are listed below. Those that are not, should be completed consistent with other rows of chemistry data. There are two sections, one for the entry of the mass per sample and one for the entry of the calculated aqueous concentration resulting from SPMDs samplers and the USGS calculator.

Mass Per Sample Entry

A row of data is the result of sorbent analysis (or accompanying quality control sample).

- Station Code Monitoring location where passive sampler was deployed
- SampleDate End date of passive sampler deployment
- EventCode "WQ"
- CollectionDepth use "-88"
- Unit Collection Depth use "m"
- LabCollectionComments Use this comment field for both the number of days the passive sampler was deployed and the mass of the sorbent in the sample (i.e. being extracted together); Example: "21 days; 400 mg of sorbent"
- CollectionMethodCode "PassiveSampler"
- SampleTypeCode "Integrated³" for environmental sample. Other SampleTypes may be appropriate for QC samples. For example, if a device using spiked sorbents is also deployed, use "FieldSp" as the SampleTypeCode for the row representing the analysis of the spiked sorbent.
- Replicate
 - If there is one sorbent exposed within a housing, the replicate number should be "1."

¹ Similar devices that do have moving parts, such as CLAM devices, are considered "active" samplers and will be addressed in separate guidance.

² One housing may include multiple sorbents that can be extracted together or separately for the same or different analytes. These business rules specify that the results be reported as mass of analyte per sample. What constitutes a sample depends on what sorbents are being extracted and analyzed together.

³ Update the description of integrated to better address passive samplers as well as depth integrated.

Chemistry Data Submission Guidance Document

Appendix D – Passive Sampler Data Entry Guidance

- If multiple sorbents are exposed to the sample medium at the same time, within the same housing, and
 - Each sorbent was extracted and analyzed for the same analyte separately, there should be a corresponding number of rows, each with a sequential replicate number, starting with "1;"
 - Each sorbent was analyzed for a different analyte, the replicate should be "1;" or
 - The same type of sorbents were extracted together and analyzed for one analyte, the replicate number should be "1."
- CollectionDeviceName Describes the passive sampler and sorbent used; request new values consistent with the following.
 - CollectionDeviceName: "[Type of device] _[sorbent]_[sorbent size without units]_[DLM⁴ status, if applicable]_[membrane pore size without units, if applicable]"
 - Example: Chemcatcher_SDB-RPS-empore_47_PES DLM_0.1
 - CollectionDeviceDescription: "Sample passively collected by [Device type] Sampler. Extraction sorbent – [sorbent material and size with units]. Diffusion limiting membrane: [DLM substance/none], [membrane pore size with units, if applicable]"
 - Example: Sample passively collected by Chemcatcher Sampler. Extraction sorbent - Styrene-divinyl benzene - reversed phase sulfonate (SDB-RPS)
 Empore 47 mm disk. Diffusion limiting membrane: Polyethersulfone (PES), 0.1 um
- Matrix "Extract_Samplewater" or "Extract_PoreWater" with description: "Pore Water Extraction from sorbent media or solid phase extraction that has been exposed to sediment."⁵
- MethodName Method used to analyze filter extract
- FractionName "Dissolved"
- UnitName mass of analyte per sample (ex. ug/sample)
- MDL Record the method detection limit of the analysis
- RL Record the reporting limit of the analysis
- LabReplicate Enter according to lab analysis of extract
- PrepPreservationName At a minimum, use "FieldFiltered." If pre-conditioning was done, include that as well. Associated lookup values would be:
 - FieldFiltered
 - FieldPreconditioned, FieldFiltered,
 - LabPreconditioned, FieldFiltered,
 - FieldPreconditioned
 - LabPreconditioned, LabFiltered,
 - LabPreconditioned
- PrepPreservationDate End date/time of deployment
- DigestExtractMethod Method for extracting analyte from sorbent

Appendix D – Passive Sampler Data Entry Guidance

⁴ Diffusion Limiting Membrane: used to reduce biofouling

⁵ As of the writing of these business rules, the matrix-controlled vocabulary list contains "Extract_Sediment" that will need to be end dated.

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• DigestExtractDate – date/time that extraction from sorbent material was performed in the laboratory



Figure 1 Polar Organic Chemical Integrative Sampler (POIS) housing with four sorbents. Source: <u>https://www.cerc.usgs.gov/pubs/center/pdfdocs/pocis.pdf</u>, 3/16/2022



Figure 2. Chemcatcher Passive Sampler showing three sorbent disk housings. Source: <u>https://chemcatcher.ie/system-requirements/</u>, 3/16/2022

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Aqueous Concentration Entry

The mass per sample water volume can be entered if calculated using the <u>SPMD USGS Calculator</u>.

- Station Code Monitoring location where passive sampler was deployed.
- SampleDate End date of passive sampler deployment
- EventCode "WQ"
- LabCollectionComments number of days passive sampler was deployed. Example: "21 days"
- CollectionMethodCode "PassiveSampler"
- SampleTypeCode "Integrated⁶" for environmental sample. Other SampleTypes may be appropriate for QC samples. For example, if a device using spiked sorbents is also deployed, use "FieldSp" as the SampleTypeCode for the row representing the analysis of the spiked sorbent.
- Replicate
 - If there is one sorbent exposed within a housing, the replicate number should be "1."
 - If multiple sorbents are exposed to the sample medium at the same time, within the same housing, and
 - Each sorbent was extracted and analyzed for the same analyte separately, there should be a corresponding number of rows, each with a sequential replicate number, starting with "1;"
 - Each sorbent was analyzed for a different analyte, the replicate should be "1;" or
 - The sorbents were extracted together and analyzed for one analyte, the replicate number should be "1."
- CollectionDeviceName Passive sampler and sorbent used; request new values consistent with the following.
 - CollectionDeviceName: "[Type of device] _[sorbent]_[sorbent size without units]_[DLM⁷ status, if applicable]_[membrane pore size without units, if applicable]"
 - Example: Chemcatcher_SDB-RPS-empore_47_PES DLM_0.1
 - CollectionDeviceDescription: "Sample passively collected by [Device type] Sampler. Extraction sorbent – [sorbent material and size with units]. Diffusion limiting membrane: [DLM substance/none], [membrane pore size with units, if applicable]"
 - Example: Sample passively collected by Chemcatcher Sampler. Extraction sorbent - Styrene-divinyl benzene - reversed phase sulfonate (SDB-RPS)
 Empore 47 mm disk. Diffusion limiting membrane: Polyethersulfone (PES), 0.1 um
- Matrix effluent, porewater or samplewater⁸
- *MethodName SPMD Water Concentration Estimator v[x-y] (ex. v5-2)*
- FractionName "Dissolved"
- UnitName mass of analyte per volume of water (ex. ug/L)

⁶ Update the description of integrated to better address passive samplers as well as depth integrated.

⁷ Diffusion Limiting Membrane: used to reduce biofouling

⁸ Italicized text denotes departures from Mass Per Sample Entry

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• LabReplicate – Enter according to lab analysis of extract

- PrepPreservationName At a minimum, use "FieldFiltered." If pre-conditioning was done, include that as well. Associated lookup values would be:
 - FieldFiltered
 - FieldPreconditioned, FieldFiltered,
 - LabPreconditioned, FieldFiltered,
 - \circ FieldPreconditioned
 - LabPreconditioned, LabFiltered,
 - \circ LabPreconditioned
- PrepPreservationDate End date/time of deployment
- DigestExtractMethod Method for extracting analyte from filter
- DigestExtractDate date/time that extraction from sorbent material was performed in the laboratory