

United States
Environmental Protection
Agency

Office of Administration
Cincinnati OH 45268



Proposed Standard Format for Electronic Transmission of Analytical Chemical Measurements for Environmental Monitoring Programs

PROPOSED STANDARD FORMAT
FOR
ELECTRONIC TRANSMISSION OF ANALYTICAL CHEMICAL MEASUREMENTS
FOR
ENVIRONMENTAL MONITORING PROGRAMS

BY

Bruce Almich, Frances Fallon, Margie Edwards
Computer Services and Systems Division
Office of Administration
U.S. Environmental Protection Agency
Cincinnati, OH 45268

and

William J. Budde
Environmental Monitoring and Support Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Cincinnati, OH 45268

June, 1984

U.S. ENVIRONMENTAL PROTECTION AGENCY
CINCINNATI, OH 45268

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of names of vendors, trade names or commercial products does not constitute endorsement or recommendation for use.

CONTENTS

	<u>Page</u>
Preface	v
Acknowledgement	vi
Background and Overview	vii
Introduction	1
Tape Format	1
Record Formats	2
Analysis Types	3
Production Runs	3
Record Sequence	4
File/Record Integrity	5
Dates and Times	6
Exhibits:	
1. Format of the Run Results Header Record (Type 1)	7
2A. Format of the Run Results Data Record (Type 2)	9
2B. Format of the Run Results Deleted Data Record (Type 5)	11
2C. Format of the Run Results Sample Header Data Record (Type 6)	12
3. Format of the Run Results Runtime Data Record (Type 3)	14
4. Format of the Run Results QC Limit Record (Type 4)	15
5. Format of the Run Results Special Requirements Record (Type 7)	16
6. Format of the Sample-Independent Method Detection Limits Record (Type 8)	17

CONTENTS (cont.)

	<u>Page</u>
Appendix A. Examples of Definitions for Type 7 Records	18
Appendix B. Definitions of Various Codes	42
Appendix C. Suggested Parmeth Codes for Dioxin and General Organics CLP Programs	56
Appendix D. Data Paths	60
Appendix E. Tabular List for CLP Dioxin IFB	63
Appendix F. Data Elements for Which a Standard List of Values is to be Used	76

PREFACE

The Environmental Protection Agency is responsible for receiving and analyzing an enormous quantity of environmental monitoring data each year. Much of this data is delivered in the form of analytical laboratory results arising from the measurement of pollutants contained in samples taken from the environment. The sheer volume and diversity of this data has resulted in the need for EPA to utilize Automatic Data Processing (ADP) technologies to assist in the data gathering and analysis process. In order to fully realize the benefits of modern ADP technology, it has become necessary to develop a standard approach for the delivery of monitoring data to the Agency. This document describes the philosophy and technical details of this information standard.

EPA plans to implement and make available the appropriate computer software programs for the generation, receipt, validation, and subsequent processing of information conforming to this standard and its successors, as updates are needed. At the present time, several tasks are underway to develop and install ADP systems in laboratories to generate the data formats conforming to the standard. Work is also underway at the Agency's data center, for developing a means of automated input of data conforming to the standard into Agency databases. It is anticipated that this standard automated approach will be extended to virtually all of the Agency's monitoring efforts within the next few years.

ACKNOWLEDGEMENT

The authors gratefully acknowledge the contributions of the following individuals to this project and the preparation of this document:

Phyllis Mattio of Computer Sciences Corporation, who assisted in the systems analysis of the material.

Maridah Ahmad of Computer Sciences Corporation, who tirelessly typed repeated drafts.

Dr. Randall Shobe of the U.S. Environmental Protection Agency, Headquarters, who supplied agency perspective and management guidance.

Background and Overview

Since its creation, the Environmental Protection Agency has been directly and indirectly involved in the collection, storage, and analysis of environmental measurements data, under virtually all of the enabling legislation. This programmatic area, broadly referred to as "monitoring", has been conducted inhouse and managed under contract widely throughout the Agency, across all environmental media, analytical techniques, and parameters of measurement. Direct monitoring involvement is carried out by various inhouse sampling and analysis activities, assisted by Agency service laboratories, in Regional, Research, and Program offices. Direct activity is also managed under a number of large contract laboratory programs whose annual costs to the agency total over \$30 million. Indirect activities are conducted under the permits and compliance monitoring programs which require industries, states, and municipalities to provide environmental measurements data. Throughout all of these activities, the Automatic Data Processing (ADP) resources of the Agency have been utilized to assist in the storage and analysis of environmental monitoring data.

Before the mid 1970's, the EPA monitoring program consisted mostly of inhouse sampling and analysis activities involving only a few hundred different parameters of measurement, principally taken from air and water media. The limited number of measurement parameters and organizations involved in the monitoring effort during this era contributed to a straightforward, if not simplistic, approach to data collection, storage, and quality control. Although the Agency initiated a few ADP projects aimed at automating laboratory data collection, the majority of the related ADP effort was concentrated on the development and maintenance of large-scale finished data repositories such as STORET, and SAROAD. The vast majority of monitoring data was hand-copied from inhouse service laboratory notebooks to reporting sheets which were subsequently sent to laboratory service requestors for further analysis and storage. A portion of the monitoring data was sent from service laboratories to Regional ADP units which managed its keypunching and batch transmission to the large-scale finished data repositories. Permits and compliance monitoring data was similarly collected from the states, industries, and municipalities, with subsequent keypunching for batch transmission to appropriate large-scale databases. For a small portion of the data, machine-readable formats were available as an option, such as for states furnishing air quality monitoring data to the national air database, SAROAD. Throughout this timeframe, however, the characteristics of environmental data handling included many opportunities for errors and long delay times as the data was re-copied and passed in hand written form among the several individuals and groups involved. Many of the organizations responsible for handling the data were considerably removed from the field sampling and laboratory analytical processes, thus increasing the chance for error in data entry and processing.

Since the mid-1970's, the environmental monitoring requirements imposed upon EPA have greatly increased. This has been due to new enabling

legislation and regulatory responsibilities involving vastly increased numbers of measurement parameters, sampling sites, and media types from which samples are to be taken. The enabling legislation has provided for a number of different sources of approval of environmental sampling and analytical laboratory methodology within the Agency, with no requirement to develop commonality or avoid duplication. New data reporting requirements were introduced as a result of the mandatory Quality Assurance order of 1979. The typical environmental sample is now analyzed for hundreds of organic compounds at a cost of over \$700, compared to the previous decade when samples were quickly analyzed for a few parameters at one tenth the cost. In order to meet the vastly increased requirement for analytical laboratory processing, resources have been shifted to contract laboratory programs which account for over 90% of the current EPA total analytical service laboratory program in monitoring activities.

Automatic Data Processing (ADP) systems have not been successfully adapted to meet the greater information demands indicated above. There has been no noticeable improvement in the manner in which handwritten finished data is supplied to the Agency for review, validation, and input to the national data systems. Current requirements for delivery of data from the Superfund Office of Emergency and Remedial Response Contract Laboratory Program general organics and dioxin projects alone will result in the delivery of a 2 1/4 - inch stack of hand-copied paper reports (3 copies of a 3/4-inch stack) for each of the 40,000 estimated samples to be analyzed in the next year. The result will be a stack of 1 1/2 miles of paper to be reviewed by the Agency in the next year alone! Without ADP assistance, this will be a very difficult task to carry out. Although a number of "one-time" ADP systems have been built for entry and analysis of monitoring data from specific projects (e.g. the temporary systems built for the Office of Research and Development Love Canal monitoring project), there is presently no Agency standard system or approach for this function.

In 1983, an ADP project was initiated to standardize EPA's monitoring data elements and to capture the information in machine-readable form for input to Agency data systems. The Superfund Contract Laboratory Program was identified as the initial client office for the production implementation of this project. As a part of the initial phase of the project, it was decided to establish a long term Agency commitment to obtain monitoring data for processing in standard machine-readable form(s) at the earliest possible point in the finished data processing cycle, for electronic transmission and entry into the appropriate mainframe databases. It is necessary that this effort have a minimal impact on changes to the design and the operation of the existing Agency mainframe data systems. Through a "standard transmission format" approach, it is possible to realize the benefits of automation without the need to modify mainframe database software systems. To assure these and other project goals, Computer Services and Systems Division, Cincinnati, was charged with the long term responsibility of maintaining the standard and assisting Agency mainframe monitoring database ADP support personnel in its installation, testing, and maintenance. In addition, the Office of Research and Development,

OMSQA - EMSL - Cincinnati was assigned a lead role in the implementation efforts for software in laboratory instruments to produce datasets that meet the standard transmission format. Throughout the project, the overall philosophy and goals have been the following:

1. Provide a single, flexible information standard and efficient software that will optimally meet Agency monitoring needs, with minimal changes to existing mainframe data systems.
2. Capture the data in the field or laboratory in machine-readable form at the earliest possible point, preferably without having to be manually re-entered or re-copied if it is already in machine-readable form (e.g. on disc in a laboratory data system).
3. Capture data that must be manually entered only once, without repetitive entry. Enter this data at the location and by the person most knowledgeable as to its correctness.
4. Conduct software development necessary to meet the goals of the project, starting with the most cost-beneficial data paths. All software is to be developed in the public domain and maintained by EPA to not be vendor specific. It can therefore be implemented by all institutions and instrument vendors that supply environmental analytical results to EPA. Laboratories and other institutions who will be required to meet the standard data deliverable format can either use EPA-developed software for this purpose, or develop their own.
5. The information standard and related software will be flexible in that they can be adapted to future needs, with the addition of new record and data types as these needs arise. We expect that annual updates will be required, although table entries can be changed at anytime to meet individual program needs.
6. Avoid the transmission of redundant data, i.e. data that can be reported by a specific calculation or formula involving other data elements in the standard.
7. The standard is to be capable of handling any environmental parameter, in any media, for any method of analysis. It is also to handle the necessary delineation for analytical quality control determinations based on standard statistical control charts as well as other program-specific AQC requirements and methods.
8. The initial software to meet the standard will support data transfer on industry standard 9-track magnetic tape. The standard is, however, data media independent, and the Agency may subsequently allow delivery via other vendor-independent means, such as floppy disc, or direct telecommunications.

The material in this document comprises the proposed initial EPA standard for environmental monitoring data transmission in the following hierarchy of levels:

1. An industry-wide standard for medium of delivery: Magnetic Tape. A checksum and record sequence numbering scheme allows for future use of direct (e.g. telecommunications) transmission through a "noisy" medium with full error recognition and control.
2. An EPA-wide standard for file formats and physical data recording methods on the standard medium, to allow the tape to be read by almost all Agency mini and mainframe computer systems.
3. An EPA-wide standard for record formats of records contained within the files.
4. An EPA-wide standard for data elements contained within the records. The standard includes data element definitions which will be used as edit and validation criteria by the input software.

It is proposed that this standard be adopted and programmed for use during the next eighteen months of alpha and beta testing on an Agency-wide basis. Alpha testing will be performed under the upcoming Dioxin IFB, with a limited number of participating contract laboratories. Beta testing is planned to be performed under a larger set of Dioxin IFB labs as well as under the upcoming General Organics IFB and perhaps the upcoming Inorganics IFB. Changes and refinements can be incorporated for future releases of the standard and the supporting computer software, on a regular basis after the first system is proven and running. Please direct comments on this project to Dr. William Budde, ORD-EMSL - Cincinnati, at FTS 684-7309, or Bruce Almich, OA-Computer Services - Cincinnati, at FTS 684-7769.

Format for Analytical Results Reports on Magnetic Tape

Introduction

This paper proposes an EPA standard for media (magnetic tape) and record formats to be used in transmission of analytical results. The following points should be noted:

1. The standard describes transmission formats only. It is expected that processing systems will convert the input records into forms more convenient for storage and processing.
2. Record types 1 through 6 are currently being used in existing major Agency applications. Therefore, these formats are not subject to revision. Record type 7 provides flexibility for varying needs of different applications. Record type 8 is a tentative addition to the standard.
3. Spaces between fields permit these records to be prepared by programs written for laboratory automation systems in versions of BASIC which require this feature, as well as to be compatible with Agency standard statistical and database management systems (e.g. SAS, S2K, ADABAS, etc.).
4. Record formats are consistent with requirements for a future error-free telecommunications format.

Tape Format

1. Tapes shall be industry - standard 9-track, 800 (NRZI) or 1600 (PE) bits per inch, with no internal labels.
2. Records shall be fixed-length 80-byte records consisting of ASCII characters. If the operating system producing the record requires an end-of-record code (such as carriage return or line feed), this code shall occupy record position 80. Otherwise, position 80 shall be blank.
3. Records may optionally be combined into fixed-length blocks, with a blocksize not exceeding 4000 bytes. If the block includes a prefix or postfix supplied by the operating system in addition to the records, information about the presence and length of the prefix or postfix shall be included in the external label.
4. Records shall be in the formats specified in Exhibits 1 through 6.
5. Tapes shall consist of one or more files. Each file shall end with a tapemark. The last file on the tape shall end with two tapemarks.

6. Each tape reel shall bear one or more external labels, collectively supplying the following information: volume ID, density, blocksize, recordsize, decimal value of character in record position 80, number of files, creation date, and name, address and phone number of submitter. Individual Agency environmental monitoring programs may require additional external labels such as to provide linkage to other related data (e.g. field sampling data sheets or lab "chronicles").

Record Formats

There are eight record types in the standard, with the formats shown in Exhibits 1 to 6:

<u>Type</u>	<u>Name</u>	<u>Contents</u>	<u>Exhibit</u>
1	Run Header	Contains information pertinent to the whole run (group, batch, etc.). See run definition - next page.	1
2	Finished Results	Contains a final result on an unknown or QC sample and identifying information; calibration data is not reported on type 2.	2a
3	Runtime Data	Contains instrument readings for samples of known concentration, used in establishing the state of the instrument; mainly used for the continuous flow analyzer.	3
4	Quality Control Limits	Contains QC limits for spikes, duplicates, blanks, control standards and surrogate spikes.	4
5	Deleted	Signals a deleted record; record contents are undefined except for the record type code.	2b
6	Sample Header	Contains sample-related information for "multiple analyte" run only.	2c
7	Comments/Special	Contents defined specifically for each application. See also Appendix A.	5
8	Method Detection Limit	Contains Sample - Independent Method Detection Limit (MDL)	6

Analysis Types

The standard divides all analytical procedures into two types:

1. Singles - one aliquot of a sample produces one analytical result. Record types 1 and 2 are mandatory; other types are optional. Analytes are identified by parmeth codes. Examples: Single - channel continuous flow analyzer and single analyte atomic absorption methods.
2. Multiples - one aliquot of a sample produces more than one analytical result. Record types 1, 2 and 6 are mandatory; other types are optional. Record type 6, representing the sample, contains a parmeth code which acts as an identifying label for the list of compounds analyzed. Record type 2, representing an individual analyte, contains either a parmeth code or a CAS code (organics) and an indicator ("P" or "C") as to which code was used. The two codes may not be mixed in one run. Examples: Multi-channel continuous flow analyzer, GC/MS, and ICAP methods.

It should be noted that records which are optional in the standard may be considered mandatory in a given application (e.g. Contract Lab Program, Effluent Guidelines Program).

Production Runs

Since, under the proposed standard, a file contains the results for one production run, it is necessary to define a run in terms applicable across a wide variety of analysis types. In general, a run should represent a "group" or "batch" of samples that are processed in a continuous sequence under relatively stable conditions. Specific points characterizing a run are:

- ° Calibration - initial and continuing checks. Typically all samples in a run use the same calibration data. (There will be a few exceptions, such as isotope dilution for GC/MS, where some of the calibration information is contained in each sample.)
- ° Instrument conditions - are typically constant throughout a run. Results obtained on different instruments cannot be combined in one run.
- ° Parmeth code - (see Appendix B1). XXX will be constant. Y, Z and MN will often be constants, but are not required to be. The amount of variation allowed here differs with the nature of the analytical procedure.

The time span of a run varies with the type of analysis. Many runs for inorganic analyses take a fraction of a day. Some organic analyses, such

as GC and GC/MS, take a long time for each sample, so that the run may contain data from several work shifts.

The first record in each tape file must be record type 1, the Run Header. Positions 3-22 form an identifier for the run. After removal of blanks, this would read 8404011521GC/MS for a GC/MS run started at 3:21p.m. on April 1, 1984. The measurement type is general, and will be assigned by EPA. Similarly, the parmeth code in record type 1 is a generic representation of the parmeth codes in the run, and will have zeros in any of Y, Z and MN if there are variations. In runs completed during one work shift by one individual, the initials designate the responsible analyst. For runs which involve more than one instrument operator, it may be necessary to use the initials of a manager. In any case, the initials should indicate one individual responsible for the quality and consistency of the entire run.

Record Sequence

1. A Run Header (type 1) record must be present as the first record in the file. Further occurrences of the type 1 record in the file are not allowed.
2. In "singles" runs each type 2 record represents a sample. Record types 2 (and 3 if present) should occur in the order in which analytical results were obtained. The type 2 records for quality control items have further rules (see Appendix B, Exhibit B2, for definitions of QC types):
 - a. LD1 must occur before the corresponding LD2 record, but the two records need not be adjacent. (Similar rule for FD1 and FD2)
 - b. LDX must occur before the corresponding LD2 record and LSF/LSA record pair, but the records need not be adjacent.
 - c. LSO must occur before the LSF/LSA record pair, but the records need not be adjacent. (Similar rule for FSO and FSF/FSA)
 - d. LSD must occur before the LF1/LSA record pair, which must occur before the LF2/LSA record pair, but the records need not be adjacent.
 - e. In all cases, a record pair must be adjacent. In each case, the first record of the pair represents an actual measurement, while the second holds a known concentration value supplied by the analyst:

LSF laboratory spike - final
LSA amount added

LCM laboratory control standard
LCT theoretical concentration of standard

LS1 surrogate spike - final concentration
LS2 amount added

LFM laboratory fortified blank
LFT theoretical concentration of fortified blank

LF1 laboratory spike-final - first member
LSA amount added

LF2 laboratory spike-final - second member
LSA amount added

FSF field spike-final
FSA amount added

FCM field control standard
FCT theoretical concentration of standard

FRM field reference standard-measured
FRC field reference standard-certified

FFM field fortified blank
FFT theoretical concentration of fortified blank

3. In "multiple results" runs, each unknown or quality control sample is represented by a group composed of a type 6 record, which holds samplelevel information, followed by one type 2 record for each analyte. The QCC field of the type 6 record holds a count for the number of analytes being determined. Record pairs for surrogate spikes (LS1/LS2) may occur anywhere within the group after the type 6 record, but are not included in the analyte count for the sample. The placement rules shown for singles apply, except that each sample is now represented by a group of records, instead of one record.
4. Type 4 records, holding quality control limits which were in effect during the run, may follow the type 2 QC record (or record pair), or may be grouped at the end of the run results file. The latter is preferable.
5. Type 7 records may be defined to occupy any position except before the type 1 (header) record or between the two records of the pairs listed above in 2e.
6. Type 8 records, holding method detection limits for compounds, may be inserted after the type 2 record to which they relate, or may be grouped at the end of the run results file, following the grouped type 4 records. The latter is preferable.

File/Record Integrity

All record types shall contain the following check fields to ensure file

and record integrity:

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
74-75	2	Record sequence number within file	00-99, repeated as necessary
76-79	4	Record checksum	Four hexadecimal digits; calcula- tion algorithm to be supplied

Dates and Times

Wherever a date or time-of-day is required, the information consists of successive groups of two decimal digits each, separated by blanks. Dates are given in the order YY MM DD, and times as HH MM. Since some computers generating the date and time sequence may have difficulty producing leading zeros, these will not be required on the tape. The program reading the tape will convert leading blanks to leading zeros in all date and time fields.

Exhibit 1

Format of the Run Results Header Record (Type 1)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"1"
2	1	blank	
3-4	2	Date/time of run: Year	Positions 3 through 22 Hold the run I.D. Date/time of run is beginning of instrumental analysis.
5	1	blank	
6-7	2	Month	
8	1	blank	
9-10	2	Day	
11	1	blank	
12-13	2	Hour of Instrument Run	
14	1	blank	
15-16	2	Minute of Instrument Run	
17	1	blank	
18-22	5	Measurement Type	general; e.g. GC/MS
23	1	blank	
24-30	7	Parameter/method Identifier	Often a generic code
31	1	blank	
32-34	3	Person responsible for run	3 initials
35	1	blank	
36	1	Lab Computer backlog flag	All samples from backlog

Exhibit 1 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
37	1	Lab Computer edit flag	Analyst examined and approved results on lab computer.
38-80	43	Reserved	

Exhibit 2A

Format of the Run Results Data Record (Type 2)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"2"
2	1	blank	
3-10	8	EPA Sample I.D.	Alphanumeric left justified
11	1	blank	
12-14	3	QC code	Alphanumeric; see Exhibit B2
15	1	blank	
16	1	Parameter I.D. type	"P" = parmeth "C" = CAS
17	1	blank	
18-26	9	Parameter/Method Identifier Specific parameter code	Right justified
27	1	blank	
28-33	6	Numeric analytical result	Right justified; fixed point
34	1	blank or 'E'	or scientific notation
35-37	3	Exponent	Blank field will be interpreted as "+00"
38	1	blank	
39-46	8	Units of measure	(Left justified) Established per pro- ject by Quality Assurance Officer
47	1	blank	
48-50	3	Non-numeric result	See Exhibit B5; also called a result qua- lifier

Exhibit 2A (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
51	1	blank	
52-59	8	LDM RECNO	Copied from backlog Used only in EPA standard in-house LDM system
60	1	blank	
61-65	5	Lab Computer backlog number	Used only in EPA standard in-house LDM system
66-73	8	Parameter mnemonic	" "
74-80		Reserved	

Exhibit 2B

Format of the Run Results Deleted Data Record

(Type 5)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"5"
2-73	72	Contents undefined	
74-80		Reserved	

Note: Any record type may be logically deleted by changing Record Type field to "5". Remaining contents of record are unchanged and should be ignored by all processing software.

Exhibit 2C

Format of the Run Results Sample Header Data Record

(Type 6)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"6"
2	1	blank	
3-10	8	EPA Sample I.D.	Alphanumeric, left justified
11	1	blank	
12-14	3	Analyte count	Numeric; 1-3 decimal digits; right justified; see text
15	1	blank	
16	1	Parameter I.D. type	"p"
17-19	3	blanks	
20-26	7	Parameter/Method Identifier Specific parameter code	Right justified; must be a parmeth code
27-38	12	blank	Not used
39-46	8	Units of measure	(Left justified) Established per project by Quality Assurance Officer
47-51	5	blank	Not used
52-59	8	"NOT REQD" or blank	
60	1	blank	
61-65	5	Lab Computer backlog number	Used only in EPA standard in-house LDM system

Exhibit 2C (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
66-73	8	Parameter mnemonic	Used only in EPA standard in-house LDM system
74-80		Reserved	

Exhibit 3

Format of the Run Results Runtime Data Record (Type 3)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"3"
2-4	3	blank	
5-14	10	Known value (IF)	+X.XXXE+XX
15	1	blank	
16	1	Code type	"P", "C"
17	1	blank	
18-26	9	Parameter/method identifier	Right justified
27	1	blank	
28-37	10	Instrument signal	Lowest form available e.g. absorbance +X.XXXE+XX
38	1	blank	
39-40	2	Inst. sample code	B, S, CS, T for instr. blank, standard, check standard and timing set standard
41-80	40	Reserved	

Note: Not used for CLP

Exhibit 4

Format of the Run Results QC Limit Record (Type 4)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record Type	"4"
2	1	blank	
3-10	8	QC chart type	LSPK, LSSP, LRBL, LDUP, LCST (left justified)
11	1	blank	
12-14	3	Limit type	MIN, MAX, A, B, LWL, LCL, AVE, UCL, UWL
15	1	blank	
16	1	Code type	"P", "C"
17	1	blank	
18-26	9	Parameter/method Identifier	Right justified
27	1	blank	
28-37	10	Limit value	+X.XXXE+XX
38	1	blank	
39-46	8	Date computed	MM/DD/YY
47	1	blank	
48	1	Method for calculating limit	M = manual C = computer
49-80	34	Reserved	

Note: Not used for CLP

Exhibit 5

Format of the Run Results Special Requirements Record (Type 7)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record Type	"7"
2	1	Blank	
3-5	3	Record Descriptor	3 Alphanumeric chars.
6	1	Blank	
7 to (54+n)		Specific formats are to be defined for each application	
(55+n) to 80		Reserved	

Note 1: If Record Descriptor is '000', positions 7-56 contain a free-field comment.

Note 2: "n" equals the number of between-field blanks.

Exhibit 6

Format of the Sample-Independent Method Detection Limits Record (Type 8)

Record length: 80 bytes

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"8"
2-6	5	blanks	
7-13	7	Parameter/Method Identifier	
14	1	blank	
15-23	9	CAS No.	Right justified
24	1	blank	
25-28	4	Method Detection Limit Method	EMSL or EST
29	1	blank	
30-35	6	Detection Limit	Right justified, fixed point or scientific notation
36	1	blank or 'E'	
37-39	3	Exponent	Blank field will be interpreted as "+00"
40	1	blank	
41-48	8	Units of measure	
49	1	blank	
50-55	6	Contract-required detection limit	For blanks in CLP program; right justified, fixed point or scientific notation
56	1	blank or 'E'	
57-59	3	Exponent	Blank field will be interpreted as "+00"
60-80		Reserved	

Appendix A

Examples of Definitions for Type 7 Records

The following 16 formats have been proposed to provide additional information to meet the needs of specific Agency programs.

The relative positions of these records in the file may be summarized as follows:

<u>Follows Type</u>	<u>Record Descriptors</u>	<u>Information On</u>
1	001, 005, 006, 007, 010, 011, 012, 013, 014, 015	Run (group, batch, etc.)
2 (singles) or 6 (multiples)	003, 004, 008, 009, 016	Sample
2	002, 008, 010	Analyte
1, 2 or 6	000	Run, sample, analyte (comments)

No relative positioning is specified where multiple type 7 records follow, for example, one type 2 record in a singles run. This should be dictated by the logic of the program which prepares the tape records.

Type 7 records may be regarded as "trailer" records, supplying additional information for the type 1, 2 or 6 record they follow. All type 7 records encountered refer to the closest preceding type 1, 2 or 6 record, until another type 2 or 6 record is encountered. (In the case of record pairs, type 7's follow the second member of the pair, but will normally refer to the first member, which represents an actual measurement.)

Exhibit A-1

Type 7-001

Use: To provide additional information about the whole run (group, batch, etc.).

Position: Follows type 1

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"001"
6	1	blank	
7-12	6	Lab ID	From EPA standard list
13	1	blank	
14-21	8	Date Report Prepared	YY MM DD
22	1	blank	
23-30	8	IFB Number	e.g., CLP program codes
31	1	blank	
32-41	10	Contract Number	e.g., CLP codes
42	1	blank	
43	1	Security code	"S" = secure "U" = unsecure
44	1	blank	
45-47	3	Counter for the number of performance checks in run	1-3 decimal digits; right justified

Exhibit A-2

Type 7-002

Use: To carry a compound name - used in one local GC/MS system.

Position: Follows type 2

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
1	1	Record Type	"7"
2	1	blank	
3-5	3	Record descriptor	"002"
6	1	blank	
7-14	8	EPA Sample ID	
15	1	blank	
16-24	9	CAS no.	right justified
25	1	blank	
26-58	33	Name of compound	

Exhibit A-3

Type 7-003

Use: To provide additional information about a specific sample.

Position: Follows type 6 (multiples) or 2 (singles).

<u>Record Positions</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	space
3-5	3	Record Descriptor	"003"
6	1	blank	
7-14	8	EPA Sample ID	
15	1	blank	
16-17	2	Region or other client	Alphanumeric; left justified
18	1	blank	
19-26	8	Case number	CLP program format
27	1	blank	
28-30	3	Batch/shipment number	Alphanumeric; left justified
31	1	blank	
32-34	3	Clean-up option	"A" or "AB"; left justified
35	1	blank	
36-45	10	File Name	File name in instrument data system
46	1	blank	
47-52	6	QC report number	Alphanumeric; left justified
53	1	blank	
54-56	3	Initials of instrument operator	

Exhibit A-4

Type 7-004

Use: To describe various dates in connection with a specific sample.

Position: Follows type 6 (multiples) or 2 (singles)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record descriptor	"004"
6	1	blank	
7-14	8	EPA Sample ID	
15	1	blank	
16-23	8	Date Sample Received at Lab	YY MM DD
24	1	blank	
25-32	8	Date of Beginning of Sample Prep - Extraction prior to analysis	YY MM DD
33	1	blank	
34-41	8	Date of Instrumental analysis	YY MM DD
42	1	blank	
43-47	5	Hour, Min. of analysis	HH MM
48	1	blank	
49	1	Work shift for sample prep	"G", "D" or "S" for: graveyard, day, swing
50	1	blank	
51	1	Work shift for sample analysis	"G", "D" or "S"

Exhibit A-5

Type 7-005

Use: To describe Gas Chromatograph conditions. Covers a group of samples.

Position: Follows type 1

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"005"
6	1	blank	
7-14	8	Commercial Column name	left justified e.g. SP2330
15	1	blank	
16-19	4	Column Length in meters	e.g., 100 or 99.5 or 3.5 (right justified)
20	1	blank	
21-24	4	Column inside diameter in mm	e.g., 2 or .3 (right justified)
25	1	blank	
26-28	3	Initial Column Temp. in degrees C.	e.g., 50 or 300 (right justified)
29	1	blank	
30-33	4	Initial Temp. Holding Time in Min.	XX.Y
34	1	blank	
35-44	10	First (or only) Column Temperature Program in degrees C with @ between range and degrees C/min	e.g., 45-250 @ 8
45	1	blank	
46-48	3	Second* Column Temp in de- grees C	e.g., 250 or 350

Exhibit A-5 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
49	1	blank	
50-53	4	Second* Temp. Holding Time in Min.	XX.Y
54	1	blank	
55	1	Type of Injector	S = split L = splitless N = on column
56	1	blank	
57-58	2	Carrier Gas	standard chemical Symbol e.g. He or Ar
59	1	blank	
60-62	3	Carrier Gas flow rate in mL/min or Cm/sec	nnn
63	1	blank	
64-65	2	Units code	"ML" or "CM"
66	1	blank	
67-68	2	Number of Column Temperature Programs	Right justified

*Note: When Number of Column Temperature Programs is "1", positions 46-48 and 50-53 will hold the final column temperature and holding time, and no type 7-006 record will follow.

Exhibit A-6

Type 7-006

Use: Continuation of 7-005. Used only if multiple ramp column temperature programs are employed.

Position: Follows the type 7-005 to which it applies.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"006"
6	1	blank	
7-16	10	Second Column Temperature Program in degrees C with @ between range and degrees C/min	e.g., 45-250 @ 8
17	1	blank	
18-20	3	Third Column Temperature in degrees C	
21	1	blank	
22-25	4	Third Temperature Holding Time in min.	XX.Y
26	1	blank	
27-36	10	Third Column Temperature Program	Like positions 7-16
37	1	blank	
38-40	3	Fourth Column Temperature in degrees C	Like positions 18-20
41	1	blank	
42-45	4	Fourth Temperature Holding Time in min.	Like positions 22-25
46	1	blank	

Exhibit A-6 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
47-56	10	Fourth Column Temperature Program	Like positions 7-16
57	1	blank	
58-60	3	Fifth Column Temperature in degrees C	Like positions 18-20
61	1	blank	
62-65	4	Fifth Temperature Holding Time in min.	Like positions 22-25

Exhibit A-7

Type 7-007

Use: To describe Mass Spectrometer conditions. Covers a group of samples.

Position: Follows type 1

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"007"
6	1	blank	
7-12	6	Instrument model	See Appendix F; left justified
13	1	blank	
14-19	6	Instrument ID	e.g. GC8312; provided by contract lab; left justified; must be unique and permanent within lab
20	1	blank	
21-23	3	Scan cycle time in sec.	1.3
24	1	blank	
25-33	9	Mass Range Scanned	e.g. 50-500
34	1	blank	
35-37	3	Pos or Neg ions	"POS" or "NEG"
38	1	blank	
39-44	6	Mass Spectrometer Resolution	e.g. 500, 60000 (defined as M/delta M)
45	1	blank	
46-47	2	Ionization Mode	FA, EI, TS, CI, AP

Exhibit A-7 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
48	1	blank	
49-55	7	Reagent gas	HE or Methane or none

Exhibit A-8

Type 7-008

Use: To describe a specific ion and specific peak area or height (raw data), for a specific sample.

Position: Follows type 2 for surrogate and analyte, linked by Sample number & CAS No. Follows type 6 for internal standard. (If calibration raw data is required, could follow type 7-012, replacing 7-013.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"008"
6	1	blank	
7-14	8	EPA Sample I.D.	
15	1	blank	
16-24	9	CAS No.	Right justified
25	1	blank	
26-33	8	Ion	e.g. 320 or 320.0736 (right justified)
34	1	blank	
35-44	10	area/height	up to 10 decimal digits, right justified
45	1	blank	
46	1	Specifier for area or height	"A" or "H"
47	1	blank	
48	1	Height Measurement Method	"C" or "M" for height; blank for area

Exhibit A-9

Type 7-009

Use: To describe information on dilution factors in order to calculate final results or check contractor calculations, for a specific sample.

Position: Follows type 6

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"009"
6	1	blank	
7-14	8	EPA Sample I.D.	
15	1	blank	
16-20	5	Extract Volume in ml	e.g. 1.0 or 0.050
21	1	blank	
22-24	3	Injection Volume in uL	right justified; e.g. 50 or 0.5
25	1	blank	
26	1	Sample Units Code	"L" = liters "C" = cubic meters "K" = kilograms (wet wt.)
27	1	blank	
28-32	5	Sample Size	right justified; see note 1
33	1	blank	
34-35	2	Percent moisture	right justified
36	1	blank	
37-39	3	EGD codes for quantitation report type	CAL, EPA, PAR, STD, VER, BLK, APS

Exhibit A-9 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Record</u>
40	1	blank	
41	1	Extraction code	CLP: "J" = Jar "L" = Liquid
42	1	blank	
43	1	Concentration level	"L" = low "M" = medium "H" = high (See note 2)

Note 1: Sample Size is the volume in liters for liquids, the volume in cubic meters for air, and the wet weight in kilograms for solids. The Sample Units Code indicates which units are in use for the current sample.

Note 2: The Concentration level is an estimate of overall level for all analytes together.

Exhibit A-10

Type 7-010

Use: To describe retention time data for calibration or analytes in samples, for GC and GS/MS analyses.

Position: When Use Specifier (position 60) = "A", this record follows type 2; when Use Specifier = "C", this record follows type 7-013.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"010"
6	1	blank	
7-14	8	EPA Sample I.D.	Blank for calibration
15	1	blank	
16-24	9	Cas No., analyte	right justified
25	1	blank	
26-30	5	Scan number, analyte	1-99999 integer
31	1	blank	
32-36	5	Retention time, analyte	MM:SS
37	1	blank	
38-46	9	CAS No., internal std.	For retention time internal standard (right justified).
47	1	blank	
48-52	5	Scan number, internal std.	1-99999 integer
53	1	blank	
54-58	5	Retention time, internal std.	MM:SS

Exhibit A-10 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
59	1	blank	
60	1	Use specifier	"A" = analyte "C" = calibration
61	1	blank	
62-63	2	Score	00 to 99%; used for tentatively identi- fied compounds
64	1	blank	
65	1	Score Specifier	How score was obtain- ed; one alphabetic char; from EPA sup- plied list

Exhibit A-11

Type 7-011

Use: To act as a subhead for calibration data for GC and GC/MS analyses. One required for each point of a multipoint calibration.

Position: Follows type 1.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"011"
6	1	blank	
7-14	8	Date of Calibration	YY MM DD
15	1	blank	
16-20	5	Time of Calibration	HH MM
21	1	blank	
22	1	Type of Calibration	I = initial single point M = single point of multipoint initial calibration n(numeral) = average of n points of multi- point initial cali- bration C = continuing single point check
23	1	blank	
24-30	7	Parmeth Code	generic code (Z = 0)
31	1	blank	
32-41	10	Calibration File Name	Used in GC/MS or GC data system
42	1	blank	

Exhibit A-11 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
43-45	3	Counter for the number of analytes to follow	1-3 decimal digits; right justified
46	1	blank	
47-49	3	Injection volume in ul	right justified; e.g. 0.5 or 2

Exhibit A-12

Type 7-012

Use: To describe calibration data for GC and GC/MS analyses.

Position: Applies to a group of samples on a given day or shift - follows the appropriate type 7-011. There is at least one type 7-012 for each unique parmeth-CAS combination in the run.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"012"
6	1	blank	
7-15	9	CAS No. - Internal Standard	
16	1	blank	
17-25	9	CAS No. - Analyte or Surrogate	
26	1	blank	
27-31	5	Response Factor	XX.YY $RF = \frac{Area_A \cdot Amt_{IS}}{Area_{IS} \cdot Amt_A}$ A = analyte IS = Int. Std.
32	1	blank	
33-36	4	Amt of Internal Std Injected in nanograms (Amt _{IS})	e.g., 10 or 9999
37	1	blank	
38-41	4	Amt. of analyte Injected in nanograms (Amt _A)	e.g. 10 or 9999
42	1	blank	
43-44	2	Number of ion pairs following (on Type 7-013)	Right justified

Exhibit A-13

Type 7-013

Use: Continuation of 7-012

Position: Same as 7-012. Follows the 7-012 record to which it applies. More than one type 7-013 may follow one type 7-012.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	Blank	
3-5	3	Record descriptor	"013"
6	1	Blank	
7-14	8	First* ion used for internal standard area	e.g. 322 or 331.9875 (right justified)
15	1	Blank	
16-23	8	First* ion used for analyte area	
24	1	Blank	
25-32	8	Second* ion used for internal standard area	
33	1	Blank	
34-41	8	Second* ion used for analyte area	
42	1	Blank	
43-50	8	Third* ion used for internal standard area	
51	1	Blank	
52-59	8	Third* ion used for analyte area	

*If two 7-013 records are used after one 7-012, these fields become the fourth, fifth and sixth ions on the second record.

Exhibit A-14

Type 7-014

Use: To describe performance check (P/C) evaluation data for GC/MS analyses.

Position: Applies to a group of samples on a given day or shift - after type 7-001.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record Descriptor	"014"
6	1	blank	
7-14	8	Date of P/C	YY MM DD
15	1	blank	
16-20	5	Time of P/C	HH MM
21	1	blank	
22-29	8	Case Number	CLP program format
30	1	blank	
31-37	7	Parameter method identifier	Generic (Z = 0)
38	1	blank	
39-47	9	CAS No. - P/C compound	
48	1	blank	
49	1	Type of check	1 alphabetic char. "R" = Chromatography Resolution "M" = Mass spec. calibration of mass and abundance
50	1	blank	

Exhibit A-14 (cont.)

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
51-54	4	Chromatographic re- solution	XX.Y; X/Y*100; used, for example, for CLP dioxin program
55	1	blank	
56-57	2	Number of ion - % rel. abundance pairs following (on type 7-015)	1-2 decimal digits (right justified)

Exhibit A-15

Type 7-015

Use: Continuation of 7-014. There may be more than one type 7-015 following one 7-014 record.

Position: Follows the type 7-014 record to which it applies.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Content</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record descriptor	"015"
6	1	blank	
7-9	3	First ion	1-3 decimal digits, right justified
10	1	blank	
11-15	5	Relative abundance of first ion	XXX.Y
16-25	10	Second ion	Same format as positions 6-15
26-35	10	Third ion	
36-45	10	Fourth ion	
46-55	10	Fifth ion	
56-65	10	Sixth ion	

Note: Second type 7-015 for same 7-014 would describe seventh to twelfth ions, etc.

Exhibit A-16

Type 7-016

Format of the Sample-Dependent Method Detection Limits Record

Use: To provide the detection limit required for the CLP Dioxin program.

Position: Follow type 6.

<u>Record Position</u>	<u>Field Length</u>	<u>Field Contents</u>	<u>Remarks</u>
1	1	Record type	"7"
2	1	blank	
3-5	3	Record descriptor	"016"
6	1	blank	
7-13	7	Parameter/Method Identifier	
14	1	blank	
15-23	9	CAS No.	Right justified
24	1	blank	
25-28	4	Method Detection Limit Method	e.g. EMSL, EST, VII
29	1	blank	
30-35	6	Detection Limit	Right justified, fixed point or scientific notation
36	1	blank or 'E'	
37-39	3	Exponent	Blank field will be interpreted as "+00"
40	1	blank	
41-48	8	Units of measure	

Appendix B

Definitions of Various Codes

- Exhibit B1. Structure of the Parameter/Method (Parmeth) Code
- Exhibit B2. Definitions of Quality Control Items and Codes (QCC) in Type 2 Records
- Exhibit B3. Definitions of Quality Control Codes in Type 4 Records
- Exhibit B4. Codes for Sample Medium (Matrix, Source)
- Exhibit B5. List of Result Qualifiers

Exhibit B1

STRUCTURE OF THE PARAMETER/METHOD (PARMETH) CODE

The Parmeth Code

The parameter/method (parmeth) code is a seven character alphanumeric code that is utilized in the Agency Laboratory Data Management System. The purpose of the parmeth code is to define concisely the target analytes, the details of the method of analysis, and the sample medium which was the subject of the analysis. The parmeth code has the form:

XXXYZMN

Where:

- XXXXN defines one or more target analytes plus the analytical method. This part of the code is identical with the method numbers defined in EPA methods manuals (1) and the Federal Register (2) for water methods. If N is not specified, the default value is one. The XXXN part of the code is always numeric.
- Y is an alphanumeric modifier which specifies that an allowed option in the method has been implemented, or specifies fractions of analytes in the method. The defined values of Y are dependent on the value of XXXN, that is, a Y = 5 in the 200 series methods may have a different meaning than Y = 5 in the 300 series methods. As an example, Y may distinguish total and dissolved phosphorus measured by the same method but with or without the optional method filtration. Another example is the use of Y to distinguish the acid and base/neutral fractions in method 625. If Y is not defined in a method, the default value is one.
- Z is a code to define the environmental medium to which the analysis was applied, for example, drinking water or ambient air. The Z part of the code is alphanumeric.
- M is a numeric code to allow variations in the method that may be necessary for local needs. The M may be used, for example, to distinguish data from two similar or identical instruments running the same method in a high production laboratory. One instrument may be M = 1 and the other M = 2. This digit may also be used to define analytes in addition to those defined by XXXN. Local users are requested to use M = 0, 1, 2, 3, or 4 when M is defined in connection with an officially promulgated XXXN method. Purely local methods are M = 5-8, and M = 9 is reserved for other future uses.

The parmeth code is validated as numeric for XXX and MN and as alphanumeric for Y and Z. It is stored right justified in the 9 digit specific parameter code field.

Exhibit B2

Quality Control Items in Type 2 Records

Note: These QCC values appear in the QC code fields of type 2 records. See Exhibit 2A.

<u>QCC</u>	<u>Name</u>	<u>Definition</u>
LD1	LABORATORY DUPLICATE FIRST MEMBER	Identification of the concentration value measured from the first of two aliquots of same environmental sample. Each sample or aliquot is carried through all the same sample preanalysis processing in the laboratory that is used for unknown samples. Each aliquot is treated exactly the same throughout the laboratory analytical method. This aliquot is identified as the first member of up to nine individual aliquots. LD1 is also treated as the result for an unknown (non-AQC) sample.
LD2	LABORATORY DUPLICATE SECOND MEMBER	Identification of the concentration value measured from the second of two aliquots of the same environmental sample. Each sample or aliquot is carried through all the same sample preanalysis processing in the laboratory that is used for unknown samples. Each aliquot is treated exactly the same throughout the laboratory analytical method. This aliquot is identified as the second member of up to nine individual aliquots.
<hr/>		
LRB	LABORATORY REAGENT BLANK	Identification of a measured concentration value from a blank solution prepared from inert substances (e.g., distilled water) in the laboratory and treated exactly as a laboratory sample for the parameter being measured including all preparations, holding times, and other preanalysis treatments.
<hr/>		
LCT	LABORATORY CONTROL STANDARD - THEORETICAL	Identification of a theoretical value obtained from mathematical calculations that represents an expected concentration unbiased by real-world factors. It is calculated for a sample prepared in the lab-

oratory by dissolving a known amount of a pure compound in a known amount of clean water.

LCM LABORATORY CONTROL
STANDARD - MEASURED

Identification of the measured concentration value for a sample prepared in the laboratory by dissolving a known amount of a pure compound in a known amount of clean water. Each sample or aliquot is carried through all the same sample pre-analysis processing in the laboratory that is used for unknown samples.

LSO LABORATORY SPIKED
SAMPLE - ORIGINAL

Identification of the measured concentration value of the compound in the original environmental sample. LSO is also treated as the unknown (non-AQC) sample result.

LSA LABORATORY SPIKED
SAMPLE - SPIKE ADDED

Identification of the amount by which the concentration of the original environmental sample will increase due to the addition of the pure compound in the laboratory.

LSF LABORATORY SPIKED
SAMPLE - FINAL

Identification of the measured concentration value of the combined environmental sample and the pure compound.

$$\% \text{ Recovery} = \frac{\text{LSF} - \text{LSO}}{\text{LSA}} \times 100$$

LDX LABORATORY MULTIPLE AQC

Identification of the measured concentration value where the same root sample is used for both LD1 (1st member of duplicate) and LSO (original concentration of LAB spike), as well as an unknown (non-AQC) sample result.

LSD LABORATORY SPIKE -
DUPLICATE

Identification of the measured concentration value where the same root sample is used for independent duplicate spikes and LSO (original concentration of LAB spike) as well as an unknown (non-AQC) sample result.

LF1 LABORATORY SPIKED
SAMPLE - FINAL -
FIRST MEMBER

Identification of the measured concentration value of the combined environmental sample and the pure compound.

$$\% \text{ Recovery} = \frac{\text{LF1} - \text{LSD}}{\text{LSA}} \times 100$$

LF2	LABORATORY SPIKED SAMPLE - FINAL - SECOND MEMBER	Identification of the measured concentration value of the combined environmental sample and the pure compound. $\% \text{ Recovery} = \frac{\text{LF2} - \text{LSD}}{\text{LSA}} \times 100$
LS1	LABORATORY SURROGATE SPIKE - MEASURED	Identification of the measured concentration value of a compound added to the original environmental sample in the laboratory which is not one of the materials found in the sample.
LS2	LABORATORY SURROGATE SPIKE - ADDED	Identification of the expected or calculated concentration value of the pure compound added to the original environmental sample in the laboratory, which is not one of the materials found in the sample.
<hr/>		
LFM	LABORATORY FORTIFIED BLANK - MEASURED	Identification of the measured concentration value for a sample prepared in the laboratory by adding a known amount of a pure compound to a blank fortified with a matrix. The matrix may possibly be a man-made simulation of a naturally - occurring matrix.
LFT	LABORATORY FORTIFIED BLANK - THEORETICAL	Identification of a theoretical value obtained from mathematical calculations that represents an expected concentration unbiased by real-world factors. It is calculated for a sample prepared in the laboratory by adding a known amount of a pure compound to a blank fortified with a matrix. The matrix may possibly be a man-made simulation of a naturally - occurring matrix.
<hr/>		
LPS		Identification of a set of mass and abundance data used to confirm the presence of an analyte (mass spectroscopy only).
<hr/>		
blank		Unknown sample, not associated with quality control item.
<hr/>		
FD1	FIELD DUPLICATE - FIRST MEMBER	Identification of the concentration value measured from the first of two samples

taken at the same time and placed under identical circumstances. Each sample is treated exactly the same throughout the field and laboratory analytical methods. This audit measures scatter in the analysis step and in sample collection, preservation and holding time. This sample is identified as the first member of a duplicate pair.

FD2 FIELD DUPLICATE -
 SECOND MEMBER

Identification of the concentration value measured from the second of two samples taken at the same time and place under identical circumstances. Each sample is treated exactly the same throughout the field and laboratory analytical methods. This audit measures scatter in the analysis step and in sample collection, preservation and holding time. This sample is identified as the second member of a duplicate pair.

FRB FIELD BLANK

Identification of a measured concentration value for a blank matrix that has been prepared from inert substances (e.g., distilled water) and treated as a field sample in all aspects, including exposure to the sample bottle, holding time, preservatives and other pre-analysis treatments.

FCT FIELD CONTROL STANDARD -
 THEORETICAL

Identification of a theoretical value obtained from mathematical calculations that represents an expected concentration unbiased by real-world factors. It is calculated for a sample prepared by the requestor by dissolving a known amount of a pure compound in a known amount of clean water.

FCM FIELD CONTROL STANDARD -
 MEASURED

Identification of the measured concentration value for a sample prepared by the requestor by dissolving a known amount of a pure compound in a known amount of clean water.

FRC	FIELD REFERENCE STANDARD - CERTIFIED	Identification of the certified concentration value for a sample (submitted by the requestor) from a certification source. These samples are usually obtained from the NBS, EMSL Cincinnati, EMSL RTP, etc. Certification FRC is the "true" value.
FRM	FIELD REFERENCE STANDARD - MEASURED	Identification of the measured concentration value obtained from a sample (submitted by the requestor) having a certified value. These samples are usually obtained from the NBS, EMSL Cincinnati, EMSL RTP, etc. FRM is the laboratory "measured" value.
<hr/>		
FSO	FIELD SPIKED SAMPLE - ORIGINAL	Identification of the measured concentration value of the compound in the original environmental sample. FSO is also treated as the unknown (non-AQC) sample result.
FSA	FIELD SPIKED SAMPLE - SPIKE ADDED	Identification of the amount by which the concentration of the original environmental sample will increase due to the addition of the pure compound.
FSF	FIELD SPIKED SAMPLE - FINAL	Identification of the measured concentration value of the combined environmental sample and the pure compound. $\% \text{ Recovery} = \frac{\text{FSF} - \text{FSO}}{\text{FSA}} \times 100$
<hr/>		
FFM	FIELD FORTIFIED BLANK - MEASURED	Identification of the measured concentration value for a sample prepared in the field by adding a known amount of a pure compound to a blank fortified with a matrix. The matrix may possibly be a man-made simulation of a naturally - occurring matrix.
FFT	FIELD FORTIFIED BLANK - THEORETICAL	Identification of a theoretical value obtained from mathematical calculations that represents an expected concentration unbiased by real-world factors. It is calculated for a sample prepared in the field by adding a known amount of a pure compound to a blank fortified with a matrix. The matrix may possibly be man-made simulation of a naturally - occurring matrix.

Exhibit B3

Quality Control Codes in Type 4 Records

Note: Type 4 records are used to record the limit values which were in force during the run. They will not be used for CLP programs.

<u>Record Field</u>	<u>Code</u>	<u>Meaning</u>
QC Chart Type	LSPK	Statistical data from Laboratory Spikes
	LSSP	Statistical data from Laboratory Surrogate Spikes
	LRBL	Statistical data from Laboratory Reagent Blanks
	LDUP	Statistical data from Laboratory Duplicates
	LCST	Statistical data from Laboratory Control Standards
Limit Type	A	Critical Range (R_C) Slope
	B	Critical Range (R_C) Intercept
		Note: Upper limit for duplicates is expressed by the critical range linear equation: $R_C = AX + B$
	MIN	Minimum concentration for which duplicates limit is applicable
	MAX	Maximum concentration for which duplicates limit is applicable
	LCL	Lower control limit
	LWL	Lower warning limit
	AVE	Mean
	UWL	Upper warning limit
	UCL	Upper control limit
		Note: LCL, LWL, AVE, UWL and UCL apply to all QC chart types except LDUP

Exhibit B4

Codes For Sample Medium (Matrix, Source)

<u>Medium</u>	<u>Code</u>
All Media, Don't Know, Or Don't Care	0
Water, Type Unknown Or Not Specified	1
Drinking Water	2
Ambient Surface Water	3
Raw Wastewater	4
Primary Effluent Wastewater	5
Effluent Wastewater (Secondary - Tertiary)	6
Industrial Wastewater	7
Salt, Ocean, Or Brackish Water	8
Ground Water	9
Leachate	A
Air, Type Unknown Or Not Specified	B
Ambient Air	C
Source Or Effluent Air	D
Industrial Workroom Air	E
Solids, Type Unknown Or Not Specified	F
Bottom Sediment Or Deposit	G
Soil	H
Sludge	I
Hazardous Wastes, Dumps	J
Fish, Shellfish Tissue	K
Plants, Algae Tissue	L
Commercial Product Formulation	M

Exhibit B4 (cont.)

Gasoline	N
Waste Oils	P
Field Sampling Equipment Solvent Washings	Q
Atmospheric Deposition (Direct only)	R

Exhibit B5

LIST OF RESULT QUALIFIERS

Definition: A result qualifier (also called a non-numeric result-see Exhibit 2A) consists of 3 alphanumeric characters which act as an indicator of the fact and the reason that the subject analysis (a) did not produce a numerical result, (b) produced a numeric result but it is qualified in some respect relating to the validity of the result, or (c) produced a numeric result but for administrative reasons is not to be reported outside the laboratory. Qualifiers related to STORET remarks are indicated in the list below.

<u>Qualifier</u>	<u>Full Name</u>	<u>Definition</u>
BDL	BELOW DETECTABLE LIMITS	There was not a sufficient concentration of the parameter in the sample to exceed the lower detection limit in force at the time the analysis was performed. (No result; STORET "W" remark)
FPS	FAILED PRELIMINARY SCREENING	A preliminary screening of the sample for the subject parameter was conducted. The result of the screening indicated that it would not be useful to determine the concentration of the parameter. (No result; no STORET remark)
NSQ	NOT SUFFICIENT QUANTITY	There was not a sufficient quantity of the sample to conduct an analysis to determine the concentration of the subject parameter. (No result; no STORET remark)
LAC	LABORATORY ACCIDENT	There was an accident in the laboratory that either destroyed the sample or rendered it not suitable for analysis. (No result; STORET "O" remark)
FAC	FIELD ACCIDENT	There was an accident in the field that either destroyed the sample or rendered it not suitable for analysis. (No results; no STORET remark)
ISP	IMPROPER SAMPLE PRESERVATION	Due to improper preservation of the sample it was rendered not suitable for analysis. (No results; no STORET remark code)

<u>Qualifier</u>	<u>Full Name</u>	<u>Definition</u>
PNQ	PRESENT BUT NOT QUANTIFIED	The subject parameter was present in the sample but no quantifiable result could be determined. (No result; STORET "M" remark)
CMP	USED AS PART OF A COMPOSITE	The sample was not analyzed for the subject parameter, instead it was used as part of a composite sample. (No result; STORET "E" remark)
NAI	NOT ANALYZED DUE TO INTERFERENCE	Because of uncontrollable interference the analysis for the subject parameter was not conducted. (No result; no STORET remark)
NAR	NO ANALYSIS RESULT	There is no analysis result. The reason is unspecified. (No result; no STORET remark)
PRE	PRESUMPTIVE PRESENCE	Presumptive evidence of presence of material. (No result; STORET "N" remark)
UND	ANALYZED BUT UNDETECTED	Indicates material was analyzed for but not detected. (No result; STORET "U" remark)
FQC	FAILED QUALITY CONTROL	The analysis result is not reliable because quality control limits were exceeded when the analysis was conducted. (Result; no STORET remark; non-reportable)
RNA	RELEASE/REPORT NOT AUTHORIZED	The analysis result is not authorized (by laboratory management) for either forwarding to a National Database or presentation in Engineering tabulations (No STORET remark)
AVG	AVERAGE VALUE	Average value - used to report a range of values (STORET "A" remark)
CNT	NON-ACCEPTABLE COLONY COUNTS	Results based on colony counts outside the acceptable range. (STORET "B" remark)
CAL	CALCULATED RESULT	Calculated result. (STORET "C" remark)
FLD	FIELD MEASUREMENT	Field measurement. (STORET "D" remark)

<u>Qualifier</u>	<u>Full Name</u>	<u>Definition</u>
FEM	FEMALE SEX	In the case of species, indicates female sex. (STORET "F" remark)
KIT	FIELD KIT DETERMINATION	Value based on field kit determination - results may not be accurate. (STORET "H" remark)
EST	ESTIMATED VALUE	Present above detection limit but not quantified within expected limits of precision. (STORET "J" remark)
CAN	CANCELLED	The analysis of this parameter was cancelled and not performed. (No result; no STORET remark)
LTL	LESS THAN LOWER DETECTION LIMIT	Actual value is known to be less than value given - lower detection limit. (STORET "K" remark)
GTL	GREATER THAN UPPER DETECTION	Actual value is known to be greater than value given - upper detection limit. (STORET "L" remark)
LTC	LESS THAN CRITERIA OF DETECTION	Value reported is less than the criteria of detection (which may differ from instrument detection limits). (STORET "T" remark)
MAL	MALE SEX	In the case of species, indicates male sex. (STORET "M" remark)
UNK	UNDETERMINED SEX	In the case of species, indicates undetermined sex. (STORET "U" remark)
RET	RETURN(ED) FOR RE-ANALYSIS	The analysis result is not approved by laboratory management and re-analysis is required by the bench analyst with no change in the parameter/method code. (No STORET remark)
EER	ENTRY ERROR	The recorded value is known to be incorrect but a correct value cannot be determined to enter a correction. (No STORET remark)
REQ	REQUEUE FOR REANALYSIS	The analysis is not approved and must be re-analyzed using a different parameter/method. (No STORET remark)

<u>Qualifier</u>	<u>Full Name</u>	<u>Definition</u>
RES	RESET	This code is used to re-set a flag in the LDM Result Record after which it is discarded. (No STORET remark)
CBC	CANNOT BE CALCULATED	The calculated analysis result cannot be calculated because an operand value is qualified.
LLS	LESS THAN LOWER STANDARD	The analysis value is less than the lower quality control standard.
MPR	MIDPOINT OF RANGE	The analysis value is the midpoint value of a range of concentrations.

Appendix C

Suggested Parmeth Codes for Dioxin and General Organics

The parmeth codes in Table C-1 are suggested for use with the CLP and EGD programs for dioxin and general organics. In all of these, the Z position should be interpreted with the aid of Exhibit B4. The generic value of 1, which represents "water, type unknown or not specified", is used for water analysis. Each of these generic parmeth codes represents a group of specific codes, with Z values of 2 through 9, A or R.

Solid samples are represented by two specific codes, with Z values of G (bottom sediment or deposit) and H (soil).

Dioxin rinsate samples use the value of Q (field sampling equipment solvent washings).

The methods used by EGD are shown for water only. The list can be expanded to other matrix values if appropriate.

Each parmeth code shown occurs in a type 6 record and acts as the header for the appropriate list of organic compounds, as given in the Federal Register for the method shown in the definition column. If an additional list of tentatively identified compounds is to be reported for a given sample, a second type 6 record is used, with a different parmeth code. This record represents a different analysis on the sample, and is followed by type 2 records for each of the tentatively identified compounds.

Table C-1

Suggested Parmeth Codes for Dioxin and General Organics

Note: CD = Contract-defined list of compounds for the method
 TI = Tentatively identified compounds (in addition to CD list)

<u>XXX</u>	<u>Y</u>	<u>Z</u>	<u>MN</u>	<u>Definition</u>
608	1	1	01	Method 608 - Pesticides and PCBs - water
608	1	G	02	Method 608 - Pesticides and PCBs - sediment, low level
608	1	H	02	Method 608 - Pesticides and PCBs - soil, low level
608	1	G	03	Method 608 - Pesticides and PCBs - sediment medium level
608	1	H	03	Method 608 - Pesticides and PCBs - soil, medium level
613	1	1	01	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - water
613	1	G	01	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - sediment
613	1	H	01	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - soil
613	1	Q	01	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - rinsate
613	1	1	02	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - water - partial scan
613	1	G	02	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - sediment - partial scan
613	1	H	02	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - soil - partial scan
613	1	Q	02	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - rinsate - partial scan
613	1	1	03	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - water - high resolution scan
613	1	G	03	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - sediment - high resolution scan
613	1	H	03	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - soil - high resolution scan
613	1	Q	03	Method 613 - 2,3,7,8-Tetrachloro-dibenzo-p-dioxin - rinsate - high resolution scan
624	1	1	01	Method 624 - GC/MS - Purgeables - water, internal/external standard, CD
624	1	G	02	Method 624 - GC/MS - Purgeables - sediment, low level, CD
624	1	H	02	Method 624 - GC/MS - Purgeables - soil, low level, CD
624	1	G	03	Method 624 - GC/MS - Purgeables - sediment, medium level, CD

624	1	H	03	Method 624 - GC/MS - Purgeables - soil, medium level, CD
624	1	1	04	Method 624 - GC/MS - Purgeables - isotope dilution - water, CD
624	1	1	21	Method 624 - GC/MS - Purgeables - water, internal/external standard, TI
624	1	G	22	Method 624 - GC/MS - Purgeables - sediment, low level, TI
624	1	H	22	Method 624 - GC/MS - Purgeables - soil, low level, TI
624	1	G	23	Method 624 - GC/MS - Purgeables - sediment, medium level, TI
624	1	H	23	Method 624 - GC/MS - Purgeables - soil, medium level, TI
624	1	1	24	Method 624 - GC/MS - Purgeables - isotope dilution - water, TI
625	A	1	01	Method 625 - GC/MS - Acid Fraction - water, internal/external standard, CD
625	B	1	01	Method 625 - GC/MS - Base/Neutral Fraction - water, internal/external standard, CD
625	C	1	01	Method 625 - GC/MS - combined acid and base/neutral fractions - water, internal/external standard, CD
625	C	G	02	Method 625 - GC/MS - combined fractions - sediment, low level, CD
625	C	H	02	Method 625 - GC/MS - combined fractions - soil, low level, CD
625	C	G	03	Method 625 - GC/MS - combined fractions - sediment, medium level, CD
625	C	H	03	Method 625 - GC/MS - combined fractions - soil, medium level, CD
625	A	1	04	Method 625 - GC/MS - Acid Fraction - water, isotope dilution, CD
625	B	1	04	Method 625 - GC/MS - Base/Neutral Fraction - water, isotope dilution, CD
625	A	1	21	Method 625 - GC/MS - Acid Fraction - water, internal/external standard, TI
625	B	1	21	Method 625 - GC/MS - Base/Neutral Fraction - water, internal/external standard, TI
625	C	1	21	Method 625 - GC/MS - combined acid and base/neutral fractions - water, internal/external standard, TI
625	C	G	22	Method 625 - GC/MS combined fractions - sediment, low level, TI
625	C	H	22	Method 625 - GC/MS - combined fractions - soil, low level, TI
625	C	G	23	Method 625 - GC/MS - combined fractions - sediment, medium level, TI

625	C	H	23	Method 625 - GC/MS - combined fractions - soil, medium level, TI
625	A	1	24	Method 625 - GC/MS - Acid Fraction - water, isotope dilution, TI
625	B	1	24	Method 625 - GC/MS - Base/Neutral Fraction - water, isotope dilution, TI

Notes:

1. For each water sample, the appropriate value of Z should replace the generic value of 1.
2. If pesticides are determined by method 625, XXXY = 625P.

Appendix D

Data Paths

Exhibit D1. Management Overview of Sample and Data Flow

Exhibit D2. Manual Entry of Instrument Control Data and Instrument Generated Data

The following exhibits demonstrate the managerial activities and data flow during the life cycle of a sample. Exhibit D1 is a broad overview beginning with the sample taken in the field, through analysis, computer processing and delivery of final reports. Exhibit D2 provides listing of all data elements needed to produce the magnetic tape standard. This includes manually entered as well as machine produced data.

EXHIBIT D1 MANAGEMENT OVERVIEW OF SAMPLE AND DATA FLOW

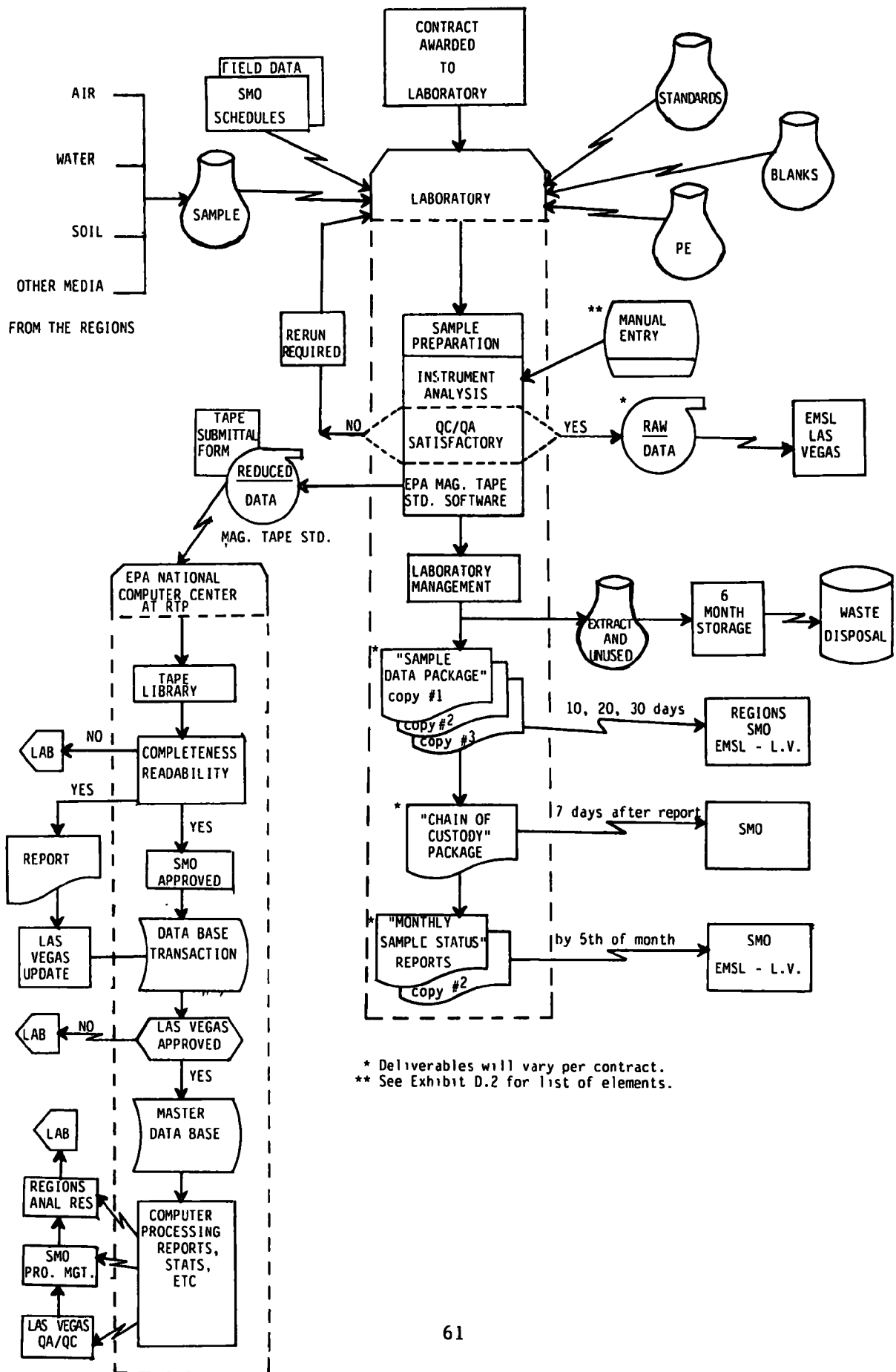


EXHIBIT D2: MANUAL ENTRY OF INSTRUMENT CONTROL DATA AND INSTRUMENT GENERATED DATA FOR AUTOMATED LAB WITH AUTOMATED INSTRUMENTS

PRE-RUN		INSTRUMENT RUN		AFTER RUN(S) / CASE		
FIXED	SELDON CHANGED	BEGINNING RUN	RUN LEVEL	LAB APPROVAL		
ELEMENTS CREATED AT START-UP	MANUAL INITIAL ENTRY BY OPERATOR ↓ MACHINE SUPPLIED STABLE ELEMENT USED FOR RUNS	MACHINE SUPPLIED	MANUAL ENTRY BY OPERATOR	MACHINE SUPPLIED	MANUAL ENTRY BY MANAGER	
*CONTRACT NO *IFB NUMBER *LAB ID *MEASUREMENT INSTR ID *PARAMETER METHOD CODES *PARAMETER METHOD ID TYPES *PARAMETER METHOD NAMES *UNITS OF MEASURE	*CALIBRATION CAS NO - ANALYTE *CALIBRATION CAS NO - INTERNAL STANDARD *CONTRACT REQUIRED METHOD DETECTION LIMIT *GC CARRIER GAS *GC CARRIER GAS FLOW RATE AND UNITS CODE *GC COLUMN LENGTH *GC COLUMN INSIDE DIAMETER *GC FIRST (OR ONLY) COLUMN TEMP PROGRAM IN DEGREES WITH BET RANGE AND DEGREES *GC COMMERCIAL COLUMN NAME *GC SECOND, THIRD, ETC COL TEMP IN DEGREES *GC SECOND, THIRD, ETC TEMP HOLDING TIME *GC INITIAL COL TEMP *GC INITIAL TEMP HOLDING TIME *GC NO OF COLUMN TEMP PROGRAMS *GC TYPE OF INJECTOR *LOCAL NAME(S) OF COMPOUNDS *METHOD DETECTION LIMIT METHOD *MS INSTR MODEL *MS INSTR ID *MS IONIZATION MODE *MS MASS RANGE SCANNED *MS MASS SPEC RESOLUTION *MS POS OR NEG IONS *MS REAGENT GAS *PC MASS (m)/CHARGE (e) *PC PARAMETER METHOD IDENTIFIERS *SPECIFIC PARAMETER METHOD CODE FOR PC COMPOUNDS *PC NUMBER OF m/e - 1 REL ABUNDANCE PAIRS *SCAN CYCLE TIME IN SEC *SPECIFIC PARAMETER METHOD CODES/ CAS CODES FOR ANALYTES	*DATE/TIME OF CALIBRATION *CALIBRATION - COUNTERS FOR NO OF ANALYTES OR PERFORMANCE CHECKS *CALIBRATION NO OF MASS (ION) NUMBER PAIRS *CALIBRATION MASS NUMBER (ION) PAIRS (INTERNAL STD AREA AND ANALYTE AREA) *CALIBRATION RETENTION TIMES FOR INTERNAL STANDARD AND ANALYTE *CALIBRATION SCAN NUMBER (ANALYTE INTERNAL STD) *CALIBRATION RESPONSE FACTOR *CALIBRATION USE SPECIFIER *DATE/TIME OF PC *DATE/TIME OF RUN *PC PAIRS OF m/e AND RELATIVE ABUNDANCE	*BATCH/SHIPMENT NO *CALIBRATION CAS AMT OF ANALYTE INJECTED *CALIBRATION AMT OF INTERNAL STD INJECTED *CALIBRATION FILE NAME *CALIBRATION SCORE SPECIFIER *CALIBRATION TYPE *CALIBRATION VOL OF ANALYTE OR INTERNAL STD INJECTED *CASE NUMBER *PC CASE NUMBER *PC CHROMATOGRAPHIC RESOLUTION *RESPONSIBLE ANALYST *DATE OF BEGINNING SAMPLE PREP-EXTRACTION PRIOR TO ANALYSIS *DATE SAMPLE RECEIVED *INITIALS OF INST OPERATOR *GC REPORT NO *REGION/CLIENT *SAMPLE ID *SAMPLE PERCENT MOISTURE *SAMPLE VOL /MT *SAMPLE UNITS CODE *SHIFT-SAMPLE PREP-EXTRACTION *WT OF DRIED SAMPLE	*ANALYTE COUNT *ANALYTICAL RESULT *AREA/HEIGHT *DATE/TIME OF SAMPLE ANALYSIS *HEIGHT MEASUREMENT METHOD *MASS (ION) NUMBER *NON-NUMERIC RESULT CODE *RETENTION TIMES ANALYTE AND REF *SCAN NUMBER *SHIFT FOR SAMPLE ANALYSIS *SPECIFIER FOR AREA OR HEIGHT	*CLEAN-UP OPTION *CONCENTRATION LEVEL *DETECTION LIMIT *E G D CODES FOR QUANT REPORT TYPE *EXTRACTION CODE *EXTRACTION VOL *FILE NAME *INJECTION VOL *NON-NUMERIC RESULT CODE *GC CODE *SCORE *SCORE SPECIFIER	*DATE REPORT PREPARED *FILE NAME *MGR INITIALS *SECURITY CODE

NOTE ELEMENTS ARE LISTED ALPHABETICALLY ORDER OF ENTRY IS NOT DETERMINED TO DATE

Appendix E

Tabular List of Data Elements for CLP Dioxin IFB

This chart presents the relationship of data elements from reports required in the Dioxin IFB (WA 84-A002) and data elements in the current EMSL Las Vegas Dioxin system as compared to the items in the EPA magnetic tape standards.

All references are to version 5 of the "U.S.E.P.A. Format for Electronic Transmission of Laboratory Analytical Chemical Measurements and Related Information".

The Raw Spectra currently delivered on magnetic tape to EMSL in Las Vegas will continue to be delivered in addition to the EPA standard magnetic tape.

The column labels in this chart are further identified as:

Data Element Name	data element name as found in required reports in the dioxin IFB (WA 84-A002) or in the current Las Vegas Dioxin System.
Report #	the form number for the reports in the IFB. Either B-1, B-2, B-3, or B-4. Las Vegas Dioxin database fields are referenced as L.V.
Standard Record Type	the record type as found in the EPA magnetic tape standard. The numerics in parenthesis represent record positions or range of positions.
Name In Standard	field contents as described in version 5 of the USEPA Magnetic Tape Standard.

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
ABSOLUTE ION ABUNDANCE	B-1 B-4	7-008 (35-44)	AREA/HEIGHT	(1) Up to 10 decimal digits, right jus- tified.
AREA/HEIGHT	L.V.			(2) Value represents the area or height under the curve generated by the instrument signal for the specified ion. (3) Refer to the following related data fields:
		7-008 (46)	AREA/HEIGHT SPECIFIER	'A' - AREA 'H' - HEIGHT
		7-008 (26-33)	ION	MASS Number specifying the ion measured.
				The following ions are required by both the IFB and Las Vegas:
				<u>Unlabeled Analyte Ions</u>
				320, 322
				<u>Surrogate Ion - 328</u>
				<u>Internal Standard Ions</u>
				332, 334
				The following ions are required by only the IFB:
				<u>Unlabeled Analyte Ions</u>
				160, 161, 194, 196, 259 324
				The type 7-007 records placement in the mag. tape standard is as follows:

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				(1) <u>Unlabeled</u> analyte ions follow type 2 record for TCDD.
				(2) <u>Surrogate</u> 328 ion follows type 2 record for surrogate.
				(3) <u>Internal std</u> 322, 334 ions follow type 6 record.
BATCH/SHIPMENT NUMBER	B-1	7-003 (28-30)	BATCH/SHIPMENT NUMBER	3 alphanumeric; assigned by SMO.
CASE NUMBER	B-1	7-003 (19-26)	CASE NUMBER	SMO or Regional office designation of a sample set from one site.
		7-014 (22-29)		8 alphanumeric
COMMENTS	B-1	7-000 (7- 56)	COMMENT	Free-field comment. Can follow any record type. 50 alphanumeric
ENTRY DATE	L.V.	---	---	Calculate as date (MM/DD/YY) mag. tape standard was processed at RTP.
EXTRA CLEANUP	B-1	7-003 (32-34)	CLEAN-UP OPTION	CLP Program Format including code for extra cleanup which is needed for IFB. 3 alphanumeric
CLEAN UP	L.V.			
COLUMN	B-1	7-005 (7- 14)	COMMERCIAL COLUMN NAME	Name of GC Column used for physically separating the analyte based on its chemical properties.
GC COLUMN	L.V.			8 alphanumeric; left justified

B-1 TCDD Data Report from Dioxin IFB

B-2 Initial Calibration Summary from Dioxin IFB

B-3 Continuing Calibration Summary from Dioxin IFB

B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB

L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
DATE	L.V.	7-001 (14-21)	DATE REPORT PREPARED	Date report is prepared. YY MM DD
REPORT DATE	B-1			
DATE	B-2 B-3	7-011 (7- 14)	DATE OF CALIBRATION	Date GC or GC/MS instru- ment was calibrated. YY MM DD
		7-011 (22)	TYPE OF CALIBRATION	Related item. Identifies the calibration point of a multipoint calibration. 1 alphanumeric I = initial single point M = single point of multi- point initial calibra- tion n(numeral) = average of n points of a multipoint initial calibration C = continuing single point check
		7-014 (7- 14)	DATE OF P/C	Date of performance check. YY MM DD
EXTRACTION	L.V.	7-009 (40)	EXTRACTION CODE	Code to specify the extraction procedure used. 1 alphabetic 'J' = Jar 'L' = Liquid
GC/MS DATE OF SAMPLE ANALYSIS	B-1 B-2 B-3	7-004 (34-41)	DATE OF IN- STRUMENT ANALYSIS	YY MM DD Date of GC/MS analysis for each sample.
ANALYTICAL DATE	L.V.			
GC/MS INSTRU- MENT ID	B-1 B-2 B-3	7-007 (14-19)	INSTRUMENT ID	6 alphanumeric, assigned by Contract lab. Left justified

B-1 TCDD Data Report from Dioxin IFB

B-2 Initial Calibration Summary from Dioxin IFB

B-3 Continuing Calibration Summary from Dioxin IFB

B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB

L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
GC/MS TIME OF SAMPLE ANALYSIS	B-1	7-004 (43-47)	HOUR, MINUTE OF ANALYSIS	HH MM Time for GC/MS analysis for each sample.
ANALYTICAL TIME	L.V.			
IFB	L.V.	7-001 (23-30)	IFB NUMBER	IFB solicitation number. 8 alphanumeric
LAB	B-1 L.V.	7-001 (7-12)	LAB ID	Code name of contracting laboratory. 6 alphanumeric
MEAN RESPONSE FACTORS - INITIAL CALIBRATION (NATIVE, SURROGATE)	B-2	---	---	Calculate the mean of each solution ID and the grand mean (mean of all solution ID's) for the analyte and for the surrogate. For each of the five solu- tion ID's for the analyte, there are three measured response factors. For each of the three solu- tion ID's (CC1,CC2,CC3) for the surrogate, there are three measured response factors.
MEAN RESPONSE FACTOR(S) - CONTINUING CALIBRATION (NATIVE, SURROGATE)	B-3	---	---	Calculate. A response factor gene- ated every 8 hours (one for the analyte and one for the surrogate) is averaged into their re- spective grand mean.
MEASURED RE- SPONSE FACTOR(S)	B-2 B-3	7-012 (27-31)	RESPONSE FACTOR	Decimal field of format of NN.NN. Calculation has already been done and may be checked by: $RF = \frac{Area_x \cdot Amt_{IS}}{Area_{IS} \cdot Amt_x}$

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				X = analyte or surrogate IS = Internal Standard
		7-012 (33-36)	AMT. OF IS INJECTED IN NANOGRAMS (AMT _{IS})	Related field, AMT _{IS}
		7-012 (38-41)	AMT. OF ANAL- YTE INJECTED IN NANOGRAMS (AMT _X)	Related field, AMT _X
		7-008 (35-40)	AREA/HEIGHT	Related field. Area of surrogate is the absolute abundance for ion 328. Area of analyte is the sum of the absolute abundance for ions 320 and 322. Area of internal standard is the sum of the abso- lute abundance for ions 332 and 334.
METHOD DETECT- ION LIMIT	B-1	7-016 (30-35)	DETECTION LIMIT	Sample-Dependent Method Detection Limit for TCDD. Fixed point or scientific notation; right justified
D.L.	L.V.	7-016 (36) (37-39)	EXPONENT	Exponent field. 'E' +NN; Blank interpreted as '+00'
PPB TCDD MEASUREMENT	B-1	2 (28-37)	NUMERIC ANALYTICAL RESULT	The concentration of 2,3,7,8-TCDD or the surrogate.
PPB SURROGATE MEASUREMENT	B-1			

B-1 TCDD Data Report from Dioxin IFB

B-2 Initial Calibration Summary from Dioxin IFB

B-3 Continuing Calibration Summary from Dioxin IFB

B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB

L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
PPB TCDD	L.V.			
		2 (34) (35-37)	EXPONENT	Exponent field. 'E' +NN; Blank interpreted as '+00'
		2 (48-50)	NON-NUMERIC RESULT (RESULT QUALIFIER)	Related field. Qualifier explaining the lack of a numeric value or qualifies the analytical result present. Std Ex- hibit B5.
ND is derived from 'BDL'.				
PERCENT RELA- TIVE ABUN- DANCE(S) - PARTIAL SCAN	B-4	---	---	Calculate. Percent Relative Abundances are calculated for ions 160, 161, 194, 196, 257, 259, 320, 322, and 324 by dividing the specific absolute ion abundance by the abundance of ion 322, then multiplying the ratio by 100.
QUALITY CONTROL SUMMARY ITEMS:	B-2 B-3	---	---	All items are to be cal- culated.
MEAN ACCURACY, SURROGATE MEASUREMENTS	B-2 B-3	---	---	Average of % accuracy for all surrogate measurements. i.e. $\frac{\%a_1 + \%a_2 + \dots + \%a_n}{n}$
# OF DATA POINTS	B-2 B-3	---	---	Number of surrogate % accuracies (n)
ACCURACY, FORTIFIED/SPIKE FIELD BLANK	B-2 B-3	---	---	$\frac{FSF}{FSA} * 100$

B-1 TCDD Data Report from Dioxin IFB

B-2 Initial Calibration Summary from Dioxin IFB

B-3 Continuing Calibration Summary from Dioxin IFB

B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB

L.V. Las Vegas Dioxin Database field

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				(See definitions in Exhibit B2)
				Note: Only 1 such sample is provided per batch for accuracy. Therefore, Sample # is the sample's ID.
RELATIVE DIFFERENCE (%), DUPLICATE ANALYSIS	B-2 B-3	---	---	$\frac{ LD1 - LD2 }{\frac{LD1 - LD2}{2}} * 100$
				(See definitions in Exhibit B2)
				Note: Only 1 sample per batch is analyzed in duplicate. Therefore, Sample # is the sample's ID.
RELATIVE ION ABUNDANCE(S)	B-1 L.V.	---	---	Calculate. Ratio of the absolute abundance of specific ions are calculated: for analyte: $\frac{\text{abs. abundance of 320}}{\text{abs. abundance of 322}}$ for internal standard: $\frac{\text{abs. abundance of 332}}{\text{abs. abundance of 334}}$
RESPONSE RATIOS PARTIAL SCAN	B-4	---	---	Calculate. Response Ratios are calculated for the following pairs by dividing the specified absolute ion abundances.

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				320/322 320/324 257/322 257/259 194/196
SAMPLE NUMBER	B-1 B-4 L.V.	2 (3-10)	EPA SAMPLE ID	Unique identifier for each sample; 8 alpha- numeric
SAMPLE #	B-2 B-3	6 (3-10)		
		7-003 (7-14)		
		7-004 (7-14)		
		7-008 (7-14)		
		7-009 (7-14)		
		2 (12-14)	QC CODE	Related field; 3 al- phanumeric; (STD Ex- hibit B2)
				For IFB and Las Vegas:
				(1) <u>Method blank</u> (MB) - derived from QC code of LRB.
				(2) <u>Partial Scan</u> (P) - derived if parameter method code (type 6 record) represents a partial scan.

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				(3) <u>Native TCDD Spike (N)</u> - derived if QC code is LDX, LSO, LSA, LSF, LSD, LF1, or LF2.
				(4) <u>Duplicate (D)</u> - derived if QC code is LDX, LD1, LD2, LD3,... or LD9.
				(5) <u>Field Blank (FB)</u> - derived from QC code FRB.
				For Las Vegas only:
				(1) <u>High Resolution (H)</u> - derived from ion on record type 7-008.
ALIQWOT WET WT. (g)	B-1	7-009 (28-32)	SAMPLE SIZE	Sample wet weight. Needs to be converted from ki- lograms to grams.
GRAMS WET WT.	L.V.			5 decimal digits; right justified
		7-009 (26)	SAMPLE UNITS CODE	Related field. Indicates the units used for the current sample. 1 alphanumeric 'L' = liters 'C' = cubic meters 'K' = kilograms (wet wt.)
SOLUTION ID	B-2 B-3			The following solution ids are derived as PC = Performance check solution CC1 = Conc. calibration solution #1 = 0.2 ug/ml

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				CC2 = Conc. calibration sol. #2 = 1.0 ug/ml CC3 = Conc. calibration sol. #3 = 5.0 ug/ml CC4 = Conc. calibration sol. #4 = 20.0 ug/ml CC5 = Conc. calibration #5 = 40.0 ug/ml
				The derivation for PC is indicated by presence of a 7-014 record. The re- maining solution ID's are derived from the amount and volume injected.
		7-011 (47-49)	INJECTION VOLUME	Related field. Volume injected in units ul.
SURROGATE PER- CENT ACCURACY (RECOVERY)	B-1 B-2 B-3			Calculate. $\frac{LS1}{LS2} * 100$
RECOVERY	L.V.			where LS1 = Analytical Result Value for measured surrogate (LS1 on type 2 re- cord) LS2 = Theoretical Value for sur- rogate (LS2 on type 2 record)
TCDD ISOMER RESOLUTION - PERCENT VALLEY	B-2 B-3	7-014 (51-54)	CHROMATO- GRAPHIC RESOLUTION	Decimal value NN.N. Already calculated by the formula: $CR = \frac{X}{Y} * 100$

B-1 TCDD Data Report from Dioxin IFB
 B-2 Initial Calibration Summary from Dioxin IFB
 B-3 Continuing Calibration Summary from Dioxin IFB
 B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB
 L.V. Las Vegas Dioxin Database fields

<u>Data Element Name</u>	<u>Report #</u>	<u>Standard Record Type</u>	<u>Name In Standard</u>	<u>Remarks</u>
				where Y = peak height X = valley height of highest valley
<hr/>				
Items required by processing but not reported in IFB or Las Vegas:				
PPB	B-1	2 (39-46)	UNITS OF MEASURE	Units of concentration for analyte or surrogate, usually 'PPB' for Dioxin.
		6 (39-46)		Default units of concentration for the method, usually 'PPB' for Dioxin.
		7-016 (41-48)		Units of concentration for the method detection limits, usually 'PPB' for Dioxin.
<hr/>				
---	---	2 (18-26)	CAS NO.	Chemical Abstracts Services Registry Number Right justified 9 numeric
		7-008 (16-24)		
		7-012 (7-15)	CAS NO. - INTERNAL STD	
		7-012 (17-25)	CAS NO. - ANALYTE OR SURROGATE	
		7-014 (39-47)	CAS NO. - P/C COMPOUND	
		7-016 (15-23)		
<hr/>				
---	---	6 (20-26)	PARAMETER/ METHOD IDENTIFIER - SPECIFIC CODE FOR GROUP	See Appendices B1 and C

B-1 TCDD Data Report from Dioxin IFB

B-2 Initial Calibration Summary from Dioxin IFB

B-3 Continuing Calibration Summary from Dioxin IFB

B-4 TCDD Data Report - Partial Scan Confirmation from Dioxin IFB

L.V. Las Vegas Dioxin Database fields

<u>Data Element</u> <u>Name</u>	<u>Report #</u>	<u>Standard</u> <u>Record Type</u>	<u>Name In</u> <u>Standard</u>	<u>Remarks</u>
------------------------------------	-----------------	---------------------------------------	-----------------------------------	----------------

7-011
(24-30)

7-014
(31-37)

B-1 TCDD Data Report
 B-2 Initial Calibration Summary
 B-3 Continuing Calibration Summary
 B-4 TCDD Data Report - Partial Scan Confirmation
 L.V. Las Vegas

Appendix F

Data Elements for Which a Standard List of Values is to be Used

<u>Record Type</u>	<u>Record Descriptor</u>	<u>Data Item</u>	<u>Value</u>
2, 6, 8		Units of measure	"PPB" for dioxin; other values to be added
8		Method Detection Limit Method (Sample - Independent)	"EML", "EST"
7	003	Clean-up option	"A" = standard cleanup "AB" = standard plus optional cleanup
7	007	Instrument model	First letter for manufacturer; 1-5 characters for model "F" = Finnegan "H" = Hewlett-Packard "K" = Kratos "V" = Varian Examples: F3100D, F3200, F3300, F3600, F4021, F4023, F4510, FTSQ, F10200, F5100, F4000, F4023T, F3200F, F4500, H5983, H5993, H5985A, H5985B, H5995A, V312MA
7	007	Ionization mode	"FA", "EI", "TS", "CI", "AP"
7	010	Score specifier	"F", "R", "P"
7	016	Method Detection Limit Method (Sample - Dependent)	"EML", "EST", "VII"
7	016	Units of measure	"PPB" for dioxin; other values to be added