ASTM INTERNATIONAL

Designation: D596 – 01 (Reapproved 2018)

Standard Guide for
Reporting Results of Analysis of Water[1]

1. Scope

1.1 This guide provides guidelines for reporting inorganic and organic results of analyses of drinking water, waste water, process water, ground water, and surface water, and so forth, to laboratory clients in a complete and systematic fashion.

1.2 The reporting of bacterial and radiological data are not addressed in this guide.

1.3 The commonly used data qualifiers for reviewing and reporting information are listed and defined. Client and laboratory specific requirements may make use of other qualifiers. This guide does not preclude the use of other data qualifiers.

1.4 This guide discusses procedures for and specific problems in the reporting of low level data, potential errors (Type I and Type II), and reporting data that are below the calculated method detection limit and above the analyte.

1.5 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D933 Practice for Reporting Results of Examination and Analysis of Water-Formed Deposits

D1129 Terminology Relating to Water

D2777 Practice for Determination of Precision and Bias of Applicable Test Methods of Committee D19 on Water

D3856 Guide for Management Systems in Laboratories Engaged in Analysis of Water

D4210 Practice for Intralaboratory Quality Control Procedures and a Discussion on Reporting Low-Level Data (Withdrawn 2002)[3]

D4460 Practice for Calculating Precision Limits Where Values are Calculated from Other Test Methods

D4840 Guide for Sample Chain-of-Custody Procedures

D5792 Practice for Generation of Environmental Data Related to Waste Management Activities: Development of Data Quality Objectives

D6091 Practice for 99 %/95 % Interlaboratory Detection Estimate (IDE) for Analytical Methods with Negligible Calibration Error

E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

3. Terminology

3.1 *Definitions:*

3.1.1 For definitions of terms used in this standard, refer to Terminology D1129.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *surrogates, n*—compounds that are similar to analytes of interest in chemical composition and behavior, separation, and measurements, but that are not normally found in environmental samples.

3.2.1.1 *Discussion*—These compounds are added to blanks, standards, samples, or spiked samples prior to analysis to confirm the proper operation of the analytical system.

3.2.2 *Type I error, n*—a statement that a substance is present when it is not.

3.2.3 *Type II error, n*—a statement that a substance was not present (was not found) when the substance was present.

4. Significance and Use

4.1 The proper use of analytical data requires adequate documentation of all inputs, that is, the source and history of the sample, laboratory performing the analysis, method of analysis, date of analysis, precision and bias of the measurements, and related quality assurance information.

4.2 In order to have defensible data, the report must be complete and accurate, providing adequate information to evaluate the quality of the data and contain supporting information that documents sampling and analysis procedures.

4.3 This guide contains some of the common data qualifiers or "flags" commonly used by laboratories following the good laboratory practices, the government contract program, or found in the commercial laboratories. Examples of these qualifiers are the use of (E) for estimated value, (U) for analyzed for but not detected, and (B) for analyte was found in the blank (see 8.11). The qualifiers included in this guide should help the laboratory and its customers to better understand each other by using standardized qualifiers.

4.4 Practice D933 is a comprehensive practice for reporting water-formed constituents such as metal oxides, acid anhydrides, and others.

5. Sample Documentation

5.1 Information regarding the source and history of the sample to be included in the analytical report should define the sample and include the following, as appropriate:

5.1.1 Laboratory performing analysis;

5.1.2 Name and address of organization or person requesting analysis;

5.1.3 Specific location of sampling and complete identification of sample;

5.1.4 Date and time of sampling;

5.1.5 Sample identification number; and

5.1.6 Sampling method, treatment, and preservation.

5.2 In addition to the information in 5.1, the following information should be included as appropriate:

5.2.1 Identification of sampling organization and individual sampler;

5.2.2 Pressure and temperature of system sampled;

5.2.3 Flow rate of water in a stream, outfall, pipe, and so forth;

5.2.4 Copies of sampling logs with signatures;

5.2.5 Chain-of-custody forms with signatures (see Guide D4840);

5.2.6 Results of field measurements; and

5.2.7 Description information (color, odor, and so forth) clearly presented.

5.2.8 The information about the sample documented in the report should be complete enough to provide direct unabridged links to underlying documents (such as chain-of-custody records and field logs) and information (such as name of sampler, lot numbers of the sample bottles, and preservatives).

6. Analysis Documentation

6.1 The laboratory system shall provide enough information to the user or reviewer so that all of the events that could influence the quality of the data can be reconstructed. The user may not need to have the information communicated directly to them, but it must be available upon request. Such information should describe how effectively all procedures were carried out and how processes were controlled so that they meet industry and government standards for performance.

6.2 As described in Guide D3856, the test method of analysis should be specified in the analytical report for each determination performed on a sample. A reference of sufficient definition or a copy of the test method should be provided to the requestor of the analytical services.

6.3 The report should note any deviation from the specified test method. Whenever a choice is allowed, the rational for selecting a given method should be documented.

6.4 The precision, bias, and detection limit of each analytical test method should be disclosed as part of either the test method or the analytical report. Consult Guide D3856 for the quality control system from which estimates of precision and bias could be made, or review the procedure for determining single-operator precision of a test method as provided in Practice D2777 for guidance. The procedure used to derive the detection limit should be identified along with any specific definitions associated with the derivation. Practice D4210 is one of many sources for computing single laboratory method detection limits. Practice D6091 provides an estimate of the detection level achievable by multiple laboratories on single sample.

6.5 The date and time on which each determination is performed should be recorded, as should other time-critical processes such as extractions, storage times, drying times, and so forth.

6.6 The analytical reports should clearly specify the form in which multi-atomic analytes, such as nitrate and orthophosphate, are reported.

6.7 If a sample is prepared for analysis in a nonstandard manner or in a manner different from the routine batch procedures (that is, special cleanup procedures or dilution required prior to analysis) then the report should clearly present the deviation and the reason why the deviation was required.

6.8 If a sample is diluted prior to analysis, the sample dilution values should be reported from which the ratios can be determined and the reason for the dilution documented.

7. Documentation of Quality

7.1 Each sample analysis may have different quality needs based on the use of the data or the data quality objectives (see Practice D5792). This information should be determined before sampling and analysis. Based on the information, an analytical report may include the following information, as appropriate:

7.1.1 Amount recovered and percent recovery of any surrogate compounds with laboratory control limits,

7.1.2 Results of corresponding check samples or blank spikes with laboratory control limits,

7.1.3 Results of analysis of duplicate samples or duplicate matrix spike samples and the percent difference with laboratory control limits,

7.1.4 Recoveries of any matrix spikes (and matrix spike duplicates) with laboratory control limits,

7.1.5 Results of all blanks,

7.1.6 Results of any reference samples run during sample analysis with laboratory control limits,