

ASTM D4128 - 06(2012) Standard Guide for Identification and Quantitation of Organic Compounds in Water by Combined Gas Chromatography and Electron Impact Mass Spectrometry

Instrument: [HP 5971A MSD with HP 5890 II GC](#)

Significance and Use

With the common occurrence in water of organic compounds, some of which are toxic, it is often necessary to identify the specific compounds present and to determine the concentration.

1. Scope

1.1 This guide covers the identification and quantitation of organic compounds by gas chromatography/mass spectrometry (GC-MS) (electron impact) that are present or extracted from water and are capable of passing through a gas chromatograph without alteration. The guide is intended primarily for solutions for which 1 ng or more of any component of interest can be introduced onto a gas chromatographic column. This guide has the advantage of providing tentative identifications of volatile and semi-volatile organics, but is restricted to (a) compounds for which reference spectra can be obtained and (b) compounds that can be separated by gas chromatography (GC). These restrictions are imposed on the guide, but are not a limitation of the technique. The guide is written for, but not restricted to, analysis using automated data acquisition and handling.

1.2 Guidelines have been included for quantitation using ASTM Test Methods [D3871](#), [D3973](#), and other GC-MS volatile/semivolatile procedures used for environmental analysis. A detection amount of 1 ng can only be considered approximate. The actual detection limits for each component must be determined in each laboratory. Actual detection amounts will vary with the complexity of the matrix, the kind and condition of the GC-MS system, the sample preparation technique chosen, and the application of cleanup techniques to the sample extract, if any. Lower levels of detection can be achieved using modern sensitive instruments or with selected ion monitoring (SIM). To determine the interlaboratory detection estimate (IDE) and the interlaboratory quantitation estimate (IQE), follow Practices [D6091](#) and [D6512](#).

1.3 The guide is applicable to the identification of many organic constituents of natural and treated waters. It includes all modes of sample introduction, including injection of organic extracts, direct aqueous injection, and purge and trap techniques.

1.4 The guide is applicable to either packed or capillary column gas chromatography, including wide-bore capillary columns. Because of their greatly enhanced resolution, capillary columns are strongly recommended.

1.5 This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.

2. Referenced Documents (*purchase separately*)

ASTM Standards

[D1066](#) Practice for Sampling Steam

D1129 Terminology Relating to Water

D1192 Guide for Equipment for Sampling Water and Steam in Closed Conduits

D1193 Specification for Reagent Water

D2908 Practice for Measuring Volatile Organic Matter in Water by Aqueous-Injection Gas Chromatography

D3370 Practices for Sampling Water from Closed Conduits

D3694 Practices for Preparation of Sample Containers and for Preservation of Organic Constituents

D3871 Test Method for Purgeable Organic Compounds in Water Using Headspace Sampling

D3973 Test Method for Low-Molecular Weight Halogenated Hydrocarbons in Water

D5175 Test Method for Organohalide Pesticides and Polychlorinated Biphenyls in Water by Microextraction and Gas Chromatography

D5316 Test Method for 1,2-Dibromoethane and 1,2-Dibromo-3-Chloropropane in Water by Microextraction and Gas Chromatography

D5317 Test Method for Determination of Chlorinated Organic Acid Compounds in Water by Gas Chromatography with an Electron Capture Detector

D5789 Practice for Writing Quality Control Specifications for Standard Test Methods for Organic Constituents

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

D6512 Practice for Interlaboratory Quantitation Estimate

E260 Practice for Packed Column Gas Chromatography

E355 Practice for Gas Chromatography Terms and Relationships

Reference: <http://www.astm.org/Standards/D4128.htm>