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Capability of detection —

Part 8: Guidance for the implementation of the ISO 11843 series

Capacité de détection —

Partie 8: Recommandations pour la mise en œuvre de la série ISO 11843

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Contents

Page

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 69, *Applications of statistical methods*, Subcommittee SC 6, *Measurement methods and results*.

A list of all parts in the ISO 11843 series can be found on the ISO website.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

0 Introduction

0.1 General

The purpose of this document is to facilitate the dissemination of the principles and methods of the ISO 11843 series on a global scale by providing a brief explanation of the background of its development, the significance of defining detection limits, the historical variation of the term detection limit, the modern concept of detection limit, and basic ideas of statistics and of each part of this series, intelligible to analytical chemists, biologists, operators, technicians, and others in various fields.

The series ISO 11843 provides statistical theories and some practical applications in a mathematically strict way. This guidance is put forth with the goal of guiding laymen in statistics in practicing the statistics of detection limits, not offering the in-depth knowledge of the relevant mathematics, but making them aware of some of the challenges of using statistical theory and the reasons for success and failure in using the formulae included in the series.

0.2 Background

The concept of detection limit was first described in 1949[1]; after that, a number of scientists submitted papers on the definition of detection limit[2][3]. Scientists in different countries have used detection limits with different definitions.

In order to avoid such global confusion, the International Union of Pure and Applied Chemistry (IUPAC) began considering the introduction of a modern detection limit using a new definition based on statistics. Representatives of the IUPAC and the International Organization for Standardization (ISO) met between 1993 and 1997 to begin efforts to develop a harmonized international chemical-metrological position on detection and quantification capabilities. The IUPAC nomenclature document was published in 1995 to help establish a uniform and meaningful approach to terminology, notation, and formulation for performance characteristics of the chemical measurement process, and in 1997 ISO published its standard (ISO 11843) for the international metrological community. IUPAC has incorporated the 1995 recommendations into its basic nomenclature volume, the Compendium on Analytical Nomenclature (IUPAC, 1998).

0.3 Parts of ISO 11843

The ISO 11843 series consists of the following published parts:

— ISO 11843-1, Capability of detection — Part 1: Terms and definitions;

— ISO 11843-2, Capability of detection — Part 2: Methodology in the linear calibration case;

— ISO 11843-3, Capability of detection — Part 3: Methodology for determination of the critical value for the response variable when no calibration data are used;

— ISO 11843-4, Capability of detection — Part 4: Methodology for comparing the minimum detectable value with a given value;

— ISO 11843-5, Capability of detection — Part 5: Methodology in the linear and non-linear calibration cases;

— ISO 11843-6, Capability of detection — Part 6: Methodology for the determination of the critical value and the minimum detectable value in Poisson distributed measurements by normal approximations;

— ISO 11843-7, Capability of detection — Part 7: Methodology based on stochastic properties of instrumental noise.

0.4 Social purposes

0.4.1 Significance of defining the minimum detectable value

The determination of the minimum detectable value is sometimes important in practical work. The value provides a criterion for deciding when “the signal is certainly not detected”, or when “the signal is significantly different from the background noise level". For example, it is valuable when measuring the presence of hazardous substances, the degree of calming of radioactive contamination, and surface contamination of semiconductor materials, as follows.

— RoHS (Restrictions on Hazardous Substances) sets limits on the use of six hazardous materials (hexavalent chromium, lead, mercury, cadmium and the flame retardant agents perbromobiphenyl, PBB, and perbromodiphenyl ether, PBDE) in the manufacturing of electronic components and related goods sold in the EU.

— Environmental pollution by radioactive materials due to accidents at nuclear power plants is a major problem. While it takes a considerable amount of time for the contaminated environment to return to its original state, it is important to monitor the state of contamination during that time.

— The condition of an analyser to be quantified when assessing the limiting performance of an instrument.

0.4.2 Trouble prevention with stakeholders

To avoid problems with stakeholders, concerning the presence or absence of hazardous substances, a kind of agreement or rule based on the scientific theory for judging the presence or absence of the hazardous substance is set up.

a) Health hazard trouble of hazardous substances.

b) Product quality assurance in commerce (non-inclusion of hazardous substances, product contamination).

0.4.3 Performance evaluation of measuring instruments

The series of ISO 11843 provides conditions for judgment on whether the detection capability of measuring instruments is adequate.

Capability of detection —

Part 8:
Guidance for the implementation of the ISO 11843 series

1 Scope

This document provides guidance for implementing the theories of the ISO 11843 series in various practical situation. As defined in this series, the term minimum detectable value corresponds to the limit of detection or detection limit defined by the IUPAC. The focus of interest is placed on the practical applications of statistics to quantitative analyses.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 11843-1, *Capability of detection — Part 1: Terms and definitions*

3 Terms, definitions and symbols

3.1 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 11843-1 apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

3.2 Symbols

X	state variable or probability density
Y	response variable
J	number of replications of measurements on the reference material representing the value of the basic state variable (blank sample)
k	constant for minimum detectable values and critical values, e.g. $x_D = k \times$ standard deviation
K	number of replications of measurements on the actual state (test sample)
N	number of replications of measurements of each reference material in assessment of the capability of detection
x	value of a state variable
y	value of a response variable