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**Water quality — Multi-compound  
class methods —**

Part 2:  
**Criteria for the quantitative  
determination of organic substances  
using a multi-compound class  
analytical method**

*Qualité de l'eau — Méthodes d'analyse de composés multi-classes —*

*Partie 2: Critères pour la détermination quantitative de composés  
organiques avec une méthode d'analyse de composés multi-classes*

ISO 21253-2:2019

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## 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](http://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](http://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 on 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 the following URL: [www.iso.org/iso/foreword.html](http://www.iso.org/iso/foreword.html).

This document was prepared by Technical Committee ISO/TC 147, *Water quality*, Subcommittee SC 2, *Physical, chemical and biochemical methods*.

A list of all parts in the ISO 21253 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](http://www.iso.org/members.html).

# Water quality — Multi-compound class methods —

## Part 2:

# Criteria for the quantitative determination of organic substances using a multi-compound class analytical method

## 1 Scope

This document specifies the criteria for developing an in-house mass spectrometry-based method for quantitative analysis of multiple subgroups of organic substances in the scope of physical-chemical analysis of water.

This document supplements ISO/TS 13530 which provides guidance on the initial characterization of the measurement performances, by providing details to select the test matrix and internal standards and criteria for analyte and internal standard recoveries.

This document is not intended as a substitute for the currently applicable analytical standards dedicated to organic compounds but as a resource bringing additional characterization elements.

## 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 8466-1, *Water quality — Calibration and evaluation of analytical methods and estimation of performance characteristics — Part 1: Statistical evaluation of the linear calibration function*

ISO 8466-2, *Water quality — Calibration and evaluation of analytical methods and estimation of performance characteristics — Part 2: Calibration strategy for non-linear second-order calibration functions*

ISO 11352, *Water quality — Estimation of measurement uncertainty based on validation and quality control data*

ISO 21253-1, *Water quality — Multi-compound class methods — Part 1: Criteria for the identification of target compounds by gas and liquid chromatography and mass spectrometry*

## 3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

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

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <http://www.electropedia.org/>

### 3.1

#### **analyte**

substance to be determined

[SOURCE: ISO/TS 28581:2012, 3.1]

### 3.2

#### **blank**

aliquot of reagent water (reagent blank) or of a matrix in which the *analyte* (3.1) is absent (matrix blank) that is treated exactly as a sample through the complete analytical procedure including extraction, clean-up, identification and quantification including all the relevant reagents and materials

Note 1 to entry: It is crucial that the laboratory specifies which blank is considered.

### 3.3

#### **calibration curve**

expression of the relation between indication and corresponding measured quantity value

[SOURCE: ISO/IEC Guide 99:2007, 4.31]

### 3.4

#### **limit of quantification**

#### **LOQ**

lowest value of a determinand that can be determined with an acceptable level of accuracy, which could be estimated by different means and shall be verified in the intended matrix

[SOURCE: ISO/TS 21231:2019, 3.2.5, modified — Note to entry has been excluded.]

### 3.5

#### **analytical method**

unambiguously written procedure describing all details required to carry out the analysis of the determinand or parameter, namely: scope and field of application, principle and/or reactions, definitions, reagents, apparatus, analytical procedures, calculations and presentation of results, performance data and test report

[SOURCE: ISO/TS 16489:2006, 3.3]

### 3.6

#### **recovery**

#### **relative recovery**

extent to which a known, added quantity of determinand in a sample can be measured by an analytical system

Note 1 to entry: Recovery is calculated from the difference between results obtained from a spiked and an unspiked aliquot of sample and is usually expressed as a percentage.

[SOURCE: ISO 5667-14:2014, 3.8]

### 3.7

#### **relative retention time**

ratio between the retention time of the target compound and the retention time of the calibration standard

[SOURCE: ISO 15680:2003, 3.5, modified — "retention-time standard" has been replaced by "calibration standard"]

### 3.8

#### **injection standard**

standard mixture added to a sample before injection into the GC-MS apparatus, to monitor variability of instrument response and to calculate internal standard recovery

Note 1 to entry: The same definition is applied for GC-MS/MS, LC-MS and LC-MS/MS.

[SOURCE: ISO 28540:2011, 3.4, modified — Note to entry has been replaced.]