

Water quality - Multi-compound class methods - Part 1:  
Criteria for the identification of target compounds by  
gas and liquid chromatography and mass spectrometry  
(ISO 21253-1:2019)

## EESTI STANDARDI EESSÕNA

## NATIONAL FOREWORD

See Eesti standard EVS-EN ISO 21253-1:2019 sisaldab Euroopa standardi EN ISO 21253-1:2019 ingliskeelset teksti.	This Estonian standard EVS-EN ISO 21253-1:2019 consists of the English text of the European standard EN ISO 21253-1:2019.
Standard on jõustunud sellekohase teate avaldamisega EVS Teatajas	This standard has been endorsed with a notification published in the official bulletin of the Estonian Centre for Standardisation.
Euroopa standardimisorganisatsioonid on teinud Euroopa standardi rahvuslikele liikmetele kättesaadavaks 02.10.2019.	Date of Availability of the European standard is 02.10.2019.
Standard on kättesaadav Eesti Standardikeskusest.	The standard is available from the Estonian Centre for Standardisation.

Tagasisidet standardi sisu kohta on võimalik edastada, kasutades EVS-i veebilehel asuvat tagasiside vormi või saates e-kirja meiliaadressile [standardiosakond@evs.ee](mailto:standardiosakond@evs.ee).

ICS 13.060.50

Standardite reprodutseerimise ja levitamise õigus kuulub Eesti Standardikeskusele

Andmete paljundamine, taastekitamine, kopeerimine, salvestamine elektroonsesse süsteemi või edastamine ükskõik millises vormis või millisel teel ilma Eesti Standardikeskuse kirjaliku loata on keelatud.

Kui Teil on küsimusi standardite autorikaitse kohta, võtke palun ühendust Eesti Standardikeskusega:  
Koduleht [www.evs.ee](http://www.evs.ee); telefon 605 5050; e-post [info@evs.ee](mailto:info@evs.ee)

The right to reproduce and distribute standards belongs to the Estonian Centre for Standardisation

No part of this publication may be reproduced or utilized in any form or by any means, electronic or mechanical, including photocopying, without a written permission from the Estonian Centre for Standardisation.

If you have any questions about copyright, please contact Estonian Centre for Standardisation:

Homepage [www.evs.ee](http://www.evs.ee); phone +372 605 5050; e-mail [info@evs.ee](mailto:info@evs.ee)

English Version

Water quality - Multi-compound class methods - Part 1:  
Criteria for the identification of target compounds by gas  
and liquid chromatography and mass spectrometry (ISO  
21253-1:2019)

Qualité de l'eau - Méthodes d'analyse de composés  
multi-classes - Partie 1: Critères pour l'identification  
des composés cibles par chromatographie en phase  
gazeuse et liquide et spectrométrie de masse (ISO  
21253-1:2019)

Wasserbeschaffenheit - Gemeinsam erfassbare  
Stoffgruppen - Teil 1: Kriterien für die Identifizierung  
von Zielverbindungen mittels Gaschromatographie und  
Flüssigchromatographie mit Massenspektrometrie-  
Kopplung (ISO 21253-1:2019)

This European Standard was approved by CEN on 9 August 2019.

CEN members are bound to comply with the CEN/CENELEC Internal Regulations which stipulate the conditions for giving this European Standard the status of a national standard without any alteration. Up-to-date lists and bibliographical references concerning such national standards may be obtained on application to the CEN-CENELEC Management Centre or to any CEN member.

This European Standard exists in three official versions (English, French, German). A version in any other language made by translation under the responsibility of a CEN member into its own language and notified to the CEN-CENELEC Management Centre has the same status as the official versions.

CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Republic of North Macedonia, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom.



EUROPEAN COMMITTEE FOR STANDARDIZATION  
COMITÉ EUROPÉEN DE NORMALISATION  
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Rue de la Science 23, B-1040 Brussels

## European foreword

This document (EN ISO 21253-1:2019) has been prepared by Technical Committee ISO/TC 147 "Water quality" in collaboration with Technical Committee CEN/TC 230 "Water analysis" the secretariat of which is held by DIN.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by April 2020, and conflicting national standards shall be withdrawn at the latest by April 2020.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. CEN shall not be held responsible for identifying any or all such patent rights.

According to the CEN-CENELEC Internal Regulations, the national standards organizations of the following countries are bound to implement this European Standard: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Republic of North Macedonia, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom.

## Endorsement notice

The text of ISO 21253-1:2019 has been approved by CEN as EN ISO 21253-1:2019 without any modification.

# Contents

Page

<b>Foreword</b>	<b>iv</b>
<b>Introduction</b>	<b>v</b>
<b>1 Scope</b>	<b>1</b>
<b>2 Normative references</b>	<b>1</b>
<b>3 Terms and definitions</b>	<b>1</b>
<b>4 Abbreviated terms</b>	<b>2</b>
<b>5 Principle</b>	<b>3</b>
<b>6 Apparatus</b>	<b>3</b>
<b>7 Identification of target compounds</b>	<b>4</b>
7.1 Procedure for identification of organic compounds with chromatography-mass spectrometry	4
7.2 Step 1: Chromatographic separation	5
7.3 Step 2: Mass spectrometric evaluation	6
7.3.1 Mass spectrometric detection	6
7.3.2 Selection of diagnostic ions	6
7.3.3 Assigning identification points	7
7.4 Step 3: Additional analytical confirmation evaluation	8
7.5 Reporting the presence of target compounds	9
7.5.1 Identification	9
7.5.2 Indication	9
7.5.3 Absence of the target compounds (<detection limit)	9
<b>8 Test report</b>	<b>9</b>
<b>Annex A (informative) Recommendations for the most commonly used techniques</b>	<b>10</b>
<b>Annex B (normative) Criteria for full scan measurement</b>	<b>12</b>
<b>Annex C (informative) Diagnostic ions to be used for identification using GC-MS<sup>n</sup> and LC-MS<sup>n</sup></b>	<b>13</b>
<b>Annex D (informative) Examples of calculating identification points</b>	<b>14</b>
<b>Bibliography</b>	<b>21</b>

## 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).

## Introduction

The use of gas chromatography (GC) and liquid chromatography (LC) in combination with mass spectrometric (MS) detection is common in many analytical standards. This detector is a powerful tool provided it is properly used. This document gives the criteria for the identification of target compounds in various types of water. This document shall be used in combination with specific analytical standards or in combination with any GC-MS and LC-MS procedure. The result of the procedure described is identified, indicated or absent.

NOTE See [Annex A](#) for recommendations for the most commonly used techniques.

This document is generally based on ISO 22892[5].

# Water quality — Multi-compound class methods —

## Part 1:

# Criteria for the identification of target compounds by gas and liquid chromatography and mass spectrometry

## 1 Scope

This document specifies the criteria for mass spectrometric identification of target compounds in water samples and is applicable to environmental samples in general. This document is intended to be used in conjunction with standards developed for the determination of specific compounds. If a standard method for analysing specific compounds includes criteria for identification, those criteria are followed.

## 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 6107 (all parts), *Water quality — Vocabulary*

## 3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 6107 (all parts) and the following 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

#### **diagnostic ion**

selected fragment ion, molecular ion or other characteristic ion from the mass spectrum of the *target compound* (3.7) with the highest possible specificity

[SOURCE: ISO 22892:2006, 3.6]

### 3.2

#### **identification point**

result of mass spectrometric investigation or other investigations/information to identify a component in environmental matrices

[SOURCE: ISO 22892:2006, 3.7]

### 3.3

#### **relative retention time**

ratio between the retention time of the *target compound* (3.7) and the retention time of the *retention time standard* (3.4)

[SOURCE: ISO 22892:2006, 3.4]