

**SLOVENSKI STANDARD**  
**oSIST prEN ISO 21253-1:2018**  
**01-december-2018**

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**Kakovost vode - Metode za več spojin - 1. del: Merila za identifikacijo ciljnih spojin s plinsko in tekočinsko kromatografijo ter masno spektrometrijo (ISO/DIS 21253-1:2018)**

Water quality - Multi-compound class methods - Part 1: Criteria for the identification of target compounds by gas and liquid chromatography and mass spectrometry (ISO/DIS 21253-1:2018)

Wasserbeschaffenheit - Multi-Class-Verfahren - Teil 1: Anleitung für die Identifizierung von Zielverbindungen durch Gas- und Flüssigchromatographie und Massenspektrometrie (ISO/DIS 21253-1:2018)

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/DIS 21253-1:2018)

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

Part 1:

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

*Qualité de l'eau — Méthodes de composés multi-class —**Partie 1: Critères pour l'identification des composés cibles par chromatographie en phase gazeuse et liquide et spectrométrie de masse*

ICS: 13.060.50

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CP 401 • Ch. de Blandonnet 8  
CH-1214 Vernier, Geneva  
Phone: +41 22 749 01 11  
Fax: +41 22 749 09 47  
Email: [copyright@iso.org](mailto:copyright@iso.org)  
Website: [www.iso.org](http://www.iso.org)

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## ISO/DIS 21253-1:2018(E)

### 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)).

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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.

## Introduction

In many analytical standards, use is made of gas chromatography (GC) and liquid chromatography (LC) in combination with mass spectrometric (MS) detection. This detector is a powerful tool provided it is properly used. In this document criteria are given for the identification of target compounds in various types of water. This document can 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.

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

The given identification criteria are in line with Commission Decision 2002/657/EC of 12 August 2002 implementing Council Directive 96/23/EC concerning performance of analytical methods and the interpretation of results. [Off. J. Eur. Commun. 2002, L221-228][6].

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# 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 gives criteria for mass spectrometric identification of target compounds in water samples and may be applied to environmental samples in general. This document shall be used in conjunction with a standard developed for the determination of the specific compounds, for example, ISO 17943<sup>[3]</sup> for volatile organic substances or ISO 16693<sup>[1]</sup> for determination of organochlorine pesticide (OCP). If the standard method for analysing specific compounds includes criteria for identification, those criteria shall be 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/DIS 21253-2, *Water quality — Multi-compound class methods — Part 2: Criteria for the quantitative determination of organic substances using a multi-compound class analytical method*

ISO/IEC 17025, *General requirements for the competence of testing and calibration laboratories*

## 3 Terms and definitions

For the purposes of this document, the terms and definitions given in the ISO 6107 series 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 with the highest possible specificity[SOURCE: ISO 22892:2006,<sup>[5]</sup> 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,<sup>[5]</sup> 3.7]

### 3.3

#### **relative retention time**

ratio between the retention time of the target compound and the retention time of the retention time standard[SOURCE: ISO 22892:2006,<sup>[5]</sup> 3.4]

**ISO/DIS 21253-1:2018(E)****3.4****retention time standard**

compound that is added to the sample (or to the sample extract) and to the calibration standard solution, and used to calculate the relative retention times of the target compounds[SOURCE: ISO 22892:2006,<sup>[5]</sup> 3.3]

**3.5****selected ion monitoring/SIM**

measurement of the intensity of selected diagnostic ions only

**3.6****standard compound**

target compound with the highest possible purity, which can be used as a reference during the analysis

Note 1 to entry: Any impurities should not have influence on the mass spectrum of the standard compound.

[SOURCE: ISO 22892:2006,<sup>[5]</sup> 3.2]

**3.7****target compound**

selected component, the presence or absence of which is being established

Note 1 to entry: This definition can also apply to a derivative of the original compound which is formed during an intentional derivatization procedure.

[SOURCE: ISO 22892:2006,<sup>[5]</sup> 3.1]

**3.8****calibration standard**

solution prepared from a secondary standard and/or stock solutions and used to calibrate the response of the instrument with respect to analyte concentration[SOURCE: ISO 18073:2004,<sup>[4]</sup> 3.1.2]

**3.9****calibration solution**

solution used to calibrate the instrument, prepared from (a) stock solution(s) or from a certified standard[SOURCE: ISO 17294-1:2004,<sup>[2]</sup> 3.4]

**4 Abbreviated terms and their meaning**

LC	Liquid chromatography
GC	Gas chromatography
MS	Mass spectrometry
GC-MS	Gas chromatography-mass spectrometry
LC-MS	Liquid chromatography-mass spectrometry
ESI	Electrospray ionization
APCI	Atmospheric pressure chemical ionization
SIM	Selected ion monitoring
SRM	Selected reaction monitoring
MRM	Multiple reaction monitoring
S/N	Signal to noise ratio

EI	Electron ionization
EI-GC-MS	Electron ionization-Gas chromatography-Mass spectrometry
CI	Chemical ionization
CI-GC-MS	Chemical ionization-Gas chromatography-Mass spectrometry
HRMS	High resolution mass spectrometry
FWHM	Full width at half maximum
MS- MS <sup>n</sup>	Mass spectrometry-Mass spectrometry
mDA	milliDalton
OCP	Organo chlorine pesticides
PCB	Polychlorinated biphenyls
PAH	Polycyclic aromatic hydrocarbons
LR-MS	Low resolution mass spectrometry
MTBE	Methyl tertiary-butyl ether
TAME	Tertiary amyl methyl ether
ECD	Electron capture detector
PFPD	Pulsed flame photometric detector
NPD	Nitrogen-phosphorus detector
PID	Photoionization detector
UV/Vis	Ultraviolet – visible spectroscopy
<i>m/z</i>	Mass to charge ratio

## 5 Principle

A target compound is identified if the measured values meet the criteria specified in this document or in the standard in which the procedures are described to analyse the target compound. Criteria are based on the relative retention times and the intensity of diagnostic ions, and other relevant factors. Additional information regarding diagnostic ions from specific international standards on the analysis of the target compound can be used. The principle of identification points is used.

## 6 Apparatus

As this document is complementary to other standards using GC-MS and LC-MS, it is assumed that the instrumentation used meets the requirements of those standards and a detailed description is not within the scope of this document. Suitable quality assurance requirements are set out in ISO/IEC 17025.