
**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 d'analyse de composés multi-classes —

*Partie 1: Critères pour l'identification de composés cibles par
chromatographie en phase gazeuse ou liquide et spectrométrie de
masse*

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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).

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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.

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.

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].

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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 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]

**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* (3.3) of the *target compounds* (3.7)

[SOURCE: ISO 22892:2006, 3.3]

**3.5
selected ion monitoring
SIM**

measurement of the intensity of selected *diagnostic ions* (3.1) only

**3.6
standard compound**

target compound (3.7) 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, 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, 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, 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, 3.4]

4 Abbreviated terms

APCI	atmospheric pressure chemical ionization
CI	chemical ionization
Da	Dalton
ECD	electron capture detector
EI	electron ionization
EI-GC-MS	electron ionization-gas chromatography-mass spectrometry
ESI	electrospray ionization

FWHM	full width at half maximum
GC	gas chromatography
GC-MS	gas chromatography-mass spectrometry
HRMS	high resolution mass spectrometry
LC	liquid chromatography
LC-MS	liquid chromatography-mass spectrometry
mDa	milliDalton
MRM	multiple reaction monitoring
MS	mass spectrometry
MS ⁿ	mass spectrometry
MTBE	methyl tertiary-butyl ether
<i>m/z</i>	mass to charge ratio
NPD	nitrogen-phosphorus detector
OCP	organo chlorine pesticides
PFPD	pulsed flame photometric detector
PID	photoionization detector
SIM	selected ion monitoring
S/N	signal to noise ratio ISO 21253-1:2019
SRM	selected reaction monitoring
TAME	tertiary amyl methyl ether
UV/Vis	ultraviolet – visible spectroscopy

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 ratio 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 (see [Annex D](#)).

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. The minimum acquisition requirements for low resolution and high resolution mass spectrometry are summarized in [Tables 1](#) and [2](#).

Table 1 — Minimum acquisition requirements for low resolution mass spectrometry

Mass range:	Peaks (masses) with a $S/N < 3$ are not taken into consideration and the lower end of the scan range is limited to 35 (to avoid the measurement of oxygen and nitrogen) to the highest mass of the target compound +10 unified atomic mass units (u) in full scan measurements.
Scan rate:	Minimum of 7 scans per peak.
Scan mode:	Full scan or SIM.
Mass resolution:	To be tuned on nominal resolution, the peak width at half-height of every tune mass should not exceed 0,7 DA.

Table 2 — Minimum acquisition requirements for high resolution mass spectrometry

Scan rate:	Minimum of 7 scans per peak.
Mass resolution:	The resolution shall be greater the 10 000 FWHM for the used mass range.
Mass accuracy:	The mass accuracy should be ≤ 5 ppm.

7 Identification of target compounds

IMPORTANT — The equipment shall be operated, and the determination shall be carried out by suitably trained staff.

7.1 Procedure for identification of organic compounds with chromatography-mass spectrometry

The procedure to qualify a component consists of three steps (see the flow scheme in [Figure 1](#)).

7.1.1 Step 1

Chromatographic evaluation (see [7.2](#)): the relative retention time shall fulfil the specified criteria.

Proceed to step 2 only if step 1 is positive.

7.1.2 Step 2

Mass spectrometric evaluation (see [7.3](#)): gathering identification points using mass spectrometric data. For qualification, the principle of identification points is used (see EN 16693^[1]).

Identification points can be obtained from mass spectrometric data, but also using other analytical information.

7.1.3 Step 3

Additional analytical confirmation evaluation (see [7.4](#)).

The following classification can be obtained.

- Identified (see [7.5.1](#)): The target compound is present in the analysed extract if at least 3 identification points are obtained.
- Indicated (see [7.5.2](#)): The target compound may be present if only 1 or 2 identification points are obtained.
- Absent (below the detection limit) (see [7.5.3](#)): No identification points are obtained using mass spectrometry.

In case the classification result "indication" is unwanted, then any result with less than 3 identification points shall be regarded as not identified.