
**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.

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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].

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]