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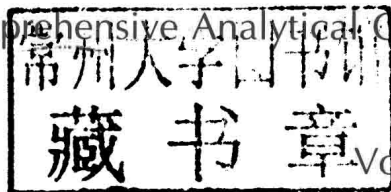
VOLUME 61

ADVANCED TECHNIQUES IN GAS  
CHROMATOGRAPHY-MASS SPECTROMETRY  
(GC-MS-MS AND GC-TOF-MS)  
FOR ENVIRONMENTAL CHEMISTRY

IMMA FERRER AND E. MICHAEL THURMAN

# Advanced Techniques in Gas Chromatography–Mass Spectrometry (GC–MS–MS and GC–TOF–MS) for Environmental Chemistry

Comprehensive Analytical Chemistry



Volume 61

Edited by

~~Imma Ferrer~~ and E. Michael Thurman

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# **Advanced Techniques in Gas Chromatography–Mass Spectrometry (GC–MS–MS and GC–TOF–MS) for Environmental Chemistry**

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## Series Editor's Preface

It is my pleasure to introduce this new volume on Advanced Techniques in Gas Chromatography-Mass Spectrometry (GC-MS-MS and GC-TOF-MS) for Environmental Chemistry, edited by Imma Ferrer and E. Mike Thurman. The reason for having such a book in the Comprehensive Analytical Chemistry series is quite obvious: I was able to convince both editors to do it. My plans to have it in the CAC series date back to my early days as Series Editor, some 15 years ago. I should add that it was not so difficult to convince Imma and Mike since both they are old friends of mine. I met Mike in person for the first time on the occasion of the 209th ACS National Meeting held in Anaheim, CA, in April 1995. Imma had just started to work in my group at that time and successfully defended her PhD thesis in December 1999.

This book can be considered complementary to other two related titles in the CAC series: Two Dimensional GC (Vol. 55 ) and TOF-MS in Food and Environmental Analysis (Vol. 58). It contains 20 chapters that cover a comprehensive variety of applications mainly in the environmental field but also in related matrices like food and biological samples. The various chapters contain details on the residue analysis of several groups of chemicals including pesticides, odour compounds, hormones, dioxins, PCBs, flame retardants and industrial applications using GC-MS-MS and/or GC-TOF-MS.

The book can be used as an academic text for postgraduate students and technicians, and as a reference for those working in chemical analytical laboratories who want to learn more about the applications of GC-tandem MS systems to environmental issues. Overall this book covers an important, routinely used and continuously improved technique in the field of Analytical Chemistry that has proven its usefulness for solving everyday problems in the analysis of organic chemical contaminants.

Finally I would like to thank both editors again and all the authors who have contributed to this book for their time and effort in preparing this excellent and useful book on GC-tandem MS techniques.

**Prof. D. Barceló**

Barcelona, Spain, July 18<sup>th</sup> 2013



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## Preface

Gas chromatography mass spectrometry (GC-MS) is not a forgotten field! Yes, it is true that LC-MS has been the preferred technique in environmental analyses over the past decade. Nonetheless, there have been major advances in the analysis of volatile and semi-volatile compounds by GC-MS. For example, there have been significant innovations in GC-MS instrumentation, such as the development of time-of-flight mass detectors (TOF) and two-dimensional gas chromatography (GC $\times$ GC) coupled to gas chromatographs. Furthermore, tandem mass spectrometry techniques (GC-MS-MS) are still commonly and successfully used for the achievement of high sensitivities.

Mainly, GC-MS techniques are used for the analysis of (i) volatile organic compounds that are analyzed by purge-and-trap techniques, (ii) semi-volatile compounds that don't ionize by LC-MS sources, and (iii) classic compounds (such as dioxins and chlorinated pesticides) where methodologies have been already well established and developed in the past. Today, even after developments for LC-MS ionization, these are still the main three areas for GC-MS applications. Furthermore, most environmental laboratories have people trained and qualified for GC-MS method development. Also, the inexpensive cost of this technique has made it easily available to all government, university, private, and industry labs. Standard methods by the Environmental Protection Agency (US EPA) have been the classic methods of choice by many scientists in the environmental field of research. Another fundamental aspect of GC-MS applications is the development of new sample preparation procedures, including extraction techniques and derivatization methods. This has opened a whole new area of remarkable applications in the field of environmental chemistry research.

Advances in high-resolution and accurate mass analysis by LC-MS have been recently carried over into the GC-MS instrumentation with time-of-flight mass spectrometry. This has only happened in the past 3–5 years, an important factor to take into account. These developments have resulted in innovative applications to environmental problems, as the reader will discover in this book.

The book consists of 20 chapters divided in two parts. The first one deals with both classic and advanced GC-MS and GC-MS-MS applications in the environmental field. The second part describes several applications using high-resolution and accurate mass GC-MS. The first part emphasizes basic features such as sample preparation for GC-MS analysis (Chapters 2, 5, and 8), development of multiresidue methods in food and water (Chapters 1, 3, and 7), analysis

of biological samples (Chapters 6 and 9), air samples (Chapter 4), and water samples (Chapters 9 and 10). The second part focuses on the use of high-resolution and time-of-flight GC-MS, describing and reviewing a whole variety of methodologies for the detection of environmental compounds. The basic principles for time-of-flight (TOF) analysis are described in detail in Chapters 11 and 12. New innovations such as the development of a miniaturized GC-TOF-MS system are illustrated in Chapter 13. Likewise, new developments in soft ionization sources are shown in Chapter 14. Several applications using high-resolution GC-MS techniques are described in Chapters 15 through 19. These applications include the analysis of stable isotopes in fracking waters, halogenated flame retardants, industrial compounds, persistent organic pollutants, and dioxins. Finally, Chapter 20 introduces a new idea called “exposomics” which discusses how GC-TOF-MS can be used to measure changes in specific individuals due to the exposure to a wide range of environmental contaminants. All classes of environmentally relevant compounds are represented in this book such as pesticides, odor-causing compounds, pharmaceuticals and personal care products, polychlorinated dibenzo-*p*-dioxins and furans, polychlorinated biphenyls, polycyclic aromatic hydrocarbons, hormones, phytoestrogens, pyrethroids, hydrocarbon gases and their stable isotopes, halogenated flame retardants, and persistent organic pollutants.

As this is our third book together, we have the tradition of predicting future trends in environmental mass spectrometry: (i) GC-MS will continue to be a popular and highly used analytical technique for the identification of volatile and semi-volatile compounds, (ii) high-resolution and time-of-flight mass spectrometry will become more and more important for nontarget and unknown analyses, gaining terrain in many environmental labs, and (iii) development of new soft ionization techniques will be the key to more effective MS-MS analyses.

Finally, we would like to acknowledge our friend, colleague, and Series Editor, Damià Barceló, for giving us the opportunity to put this book together. As always, it has been an enjoyable endeavor to be part of. And we want to thank each of the individual authors for their outstanding contributions that made possible this state-of-the-art book on GC-MS applications for environmental chemistry.

**Imma Ferrer and Mike Thurman**  
July 2013, Boulder, Colorado

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