

**HANDBOOK OF MASS
SPECTROMETRY**

UNCORRECTED PROOF

To

**WILEY SERIES ON PHARMACEUTICAL SCIENCE
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AND METHODS**

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HANDBOOK OF MASS SPECTROMETRY

**EDITED BY
MIKE S. LEE**

Wiley Series on Pharmaceutical Science and Biotechnology:
Practices, Applications and Methods

 **WILEY**

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To

FOREWORD

It is a pleasure to provide this foreword to the *Handbook of Mass Spectrometry*, edited by Dr. Mike S. Lee, a PhD graduate of my research group at the University of Florida 25 years ago. Mike is not only an outstanding scientist and a visionary in how mass spectrometry can drive science in a diverse range of disciplines; he is also a master at assembling and leading a team of experts, as he has ably demonstrated with this volume.

Mass spectrometry, although barely a hundred years old, has become the dominant force in modern analytical chemistry. It provides unparalleled levels of sensitivity and selectivity for trace analysis, and an impressive range of capabilities and application. Some of these unique capabilities arise from the unique feature of mass spectrometry (compared to other spectrometric methods) that the sample itself (matter) passes through the spectrometer and is separated and detected. Thus mass spectrometry is both a spectrometric method and a separation method!

Many of the capabilities of modern mass spectrometry arise from the remarkable advances in instrumentation over the past 30 years, many of which are reviewed in this handbook. Advances in ionization techniques have expanded the applicability of mass spectrometry from small, volatile, and thermally stable molecules to large, nonvolatile, and labile molecules, including intact proteins and polymers. The coupling of mass spectrometry with separation techniques (gas chromatography [GC], liquid chromatography [LC], capillary electrophoresis [CE], and even a second stage of mass spectrometry) has established it as the standard for trace mixture analysis. Innovations in mass analyzers continue to bring improved performance in terms of mass resolution, mass range, and sensitivity. And perhaps most impressively, the pace of advances in mass spectrometry instrumentation and methodologies has not slacked off—we continue to see remarkable advances every year.

I often date the “coming of age” of modern analytical mass spectrometry to a 1982 quote from *Chemical & Engineering News*:

Mass spectrometry has advanced to the point that it's no longer (as has been said) . . . “the method of choice – if there's no other way.”

Indeed, mass spectrometry is *the* method of choice for an amazing range of applications, from structure determination of proteins to forensic toxicology, from fundamental studies of reaction kinetics to imaging tissues. And that breadth of use and dominance of mass spectrometry is well represented in the chapters assembled here.

The remarkable growth of mass spectrometry is well represented in the growth of attendance at the Annual Meeting on Mass Spectrometry and Allied Topics of the American Society for Mass Spectrometry, from 700 attendees in the mid-1970s to 7000 today. This reflects not only the expanding scope of application of the technique, but also the ease with which modern mass spectrometers can be mastered by users new to the field, without needing to understand the underlying fundamentals. This handbook provides in its 13 sections and 52 chapters an excellent overview of that wide range of applications. The breadth of coverage makes this an excellent resource for practicing mass spectrometrists as well as to those new to the field.

Welcome to a hopefully stimulating journey through modern mass spectrometry and its breadth of applications!

RICHARD A. YOST

University of Florida
October 2011

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To

PREFACE

Mass spectrometry is an integral part of modern research in academic, industrial, and clinical laboratories. The *Handbook of Mass Spectrometry* represents the current state-of-the-art practices in these laboratory settings. The purpose of the handbook is to provide a unique reference that allows for easy access to a variety of applications that involve mass spectrometry. The intent of the handbook is to provide a resource for beginners, practitioners, and experts to obtain vital background, current approaches, and real-world methodology. Further, the handbook can also be viewed as an interactive time capsule to perhaps delineate “where we are,” “where we came from,” and “where we are headed” with regard to these specific applications—current and emerging. Thus, the handbook is not intended to be comprehensive, but rather to provide unique, in-depth information on specific techniques and experiences.

The evolution of mass spectrometry has been both dramatic and fascinating. Trace analytical measurement, specifically the demand for trace mixture analysis, has created an increased demand for this powerful tool. In many cases, the preference for the trace mixture sample type has transformed the mass spectrometer into a gold standard platform for qualitative and quantitative assays.

In its simplest form, a mass spectrometer can be viewed as a molecular weighing machine. Much like we regularly weigh ourselves in the morning to provide an early, facile benchmark for personal health and well-being, mass spectrometers are being used for a similar function. Specifically, a mass spectrometer is routinely used to monitor the “well-being” of a specific analyte. Moreover, the confirmation each analyte (structure or amount), or ensemble of analytes, often provides a sur-

rogate benchmark into a specific process that relates to a biological or chemical condition.

Regardless of the application, mass spectrometry-based methods can be organized into two areas of analytical focus: qualitative (“What is it?”) and quantitative (“How much is there?”) analysis. Similar to the building of a picture puzzle—starting with the edges (the molecular ion!) to define the size of the puzzle and/or set a defined limit to where all remaining subsequent puzzle pieces (fragment ions!) may fit inside the edges—the use of mass spectrometry provides a powerful way to quickly and confidently “define the edges” by providing molecular weight information.

Molecular weight can then become a surrogate for confirmation or even be used for the identification of a targeted compound, particularly when used in conjunction with an authentic standard or chromatographic technique, for example. Advanced studies that involve two or more dimensions of mass analysis can also be used to obtain specific structural detail (fragment ions that correspond to specific pieces of the picture puzzle!) or more selectivity to enable powerful approaches for high throughput quantitation. Moreover, similar to how high-definition televisions are improving our entertainment experience, the higher resolution mass spectrometry (and chromatography!) technologies are poised to provide a benefit to the scientific community in perhaps a highly routine manner.

Thus, the diverse contributions to the handbook are essentially unified based on the puzzle analogy. Confident and definitive “What is it?” and/or “How much is there?” information is obtained via molecular weight measurements provided by the mass spectrometer. The specific mass spectrometer and, of course,

specific chemistries (i.e., sample preparation, chromatography, ionization) help to define the analytical method.

Although the handbook is not necessarily designed to be comprehensive, the contributions represent an impressive array of critical work from diverse areas ranging from biological studies to food analysis to environmental analysis to archaeology. Each chapter in the handbook contains several compulsory elements: (1) essential background and history of the application; (2) detailed analytical methodology; and finally, (3) valuable references for more in-depth study.

Each contributor has provided critical updates in their respective field of expertise. Both current and emerging trends are highlighted. Perhaps a distinguishing feature of the handbook is that nearly all of the chapters provide a detailed description of the actual methodologies used in their respective laboratory—specifically intended so that others may initiate similar work in their respective laboratory. We hope that this unique feature will allow broad base interest and use for all scientists!

Certainly, the handbook is quite diverse in scope and application. The handbook is organized into 13 sections—starting with life sciences and culminating with specialized analytical techniques. Section I provides an exciting perspective on the recent applications of mass spectrometry for the identification of proteins and peptides. These methods represent the emerging role of mass spectrometry in biology-related fields to assist with the determination of both process and function. The section also provides the recent methodology used for imaging studies on biological systems as well as the profiling of microorganisms and viruses. The current state-of-the-art work performed in the pharmaceutical industry is featured in Section II. A continuum of work that begins with drug discovery activities such as pharmacokinetics (surrogate studies to determine dosing regimen in humans) as well as mass spectrometry methods for screening, characterization, and imaging are featured in Section II. The pharmaceutical section concludes with perspectives into drug development with the use of accelerator mass spectrometry. Exciting growth and, perhaps, a renaissance, is currently experienced in the field of clinical analysis. Section III provides a timely and critical update on the use of mass spectrometry for the screening of inborn errors and steroid analysis in a clinical laboratory setting. The distinct criteria and features necessary for a clinical laboratory—as opposed to a research setting—are powerfully represented and easily understood. Forensics is indeed a challenging area of focus that requires diverse analytical tools as well as a strict protocol of analysis—from sampling to preparation to analysis to reporting. Section

IV contains two important applications of mass spectrometry in this field. The use of isotope ratio mass spectrometry is highlighted followed by a specific application that describes the analysis of the explosive triacetone triperoxide. Section V addresses the important role of mass spectrometry in programs involved with space exploration. A fascinating perspective on the use of mass spectrometry for solar system exploration is provided. This chapter is followed by work that features the use of gas chromatography (GC)/gas chromatography–mass spectrometry (GC-MS) for the characterization of extraterrestrial organic matter. Travel and safety has been greatly impacted over the past decade. Section VI contains the recent work that describes the various uses of mass spectrometry for homeland security. Specific methods are detailed along with the requirements and challenges for this specialized application. The safety of our food and subsequent food supply is of critical worldwide importance. The role of mass spectrometry for food analysis is highlighted in Section VII. A perspective on agriculture, food and flavors is provided to give the reader some historical perspectives and background in food analysis. The recent mass spectrometry application of “top-down” proteomic methods for the identification of biomarkers of foodborne pathogens highlights future direction and analysis formats. Perhaps a cornerstone of commercial applications of mass spectrometry is in the field of environmental analysis. Section VIII contains the recent work that details how mass spectrometry is used to monitor targeted analytes such as fungicides, commercial by-products, and targeted carcinogens. Section IX focuses on geology. In this section, the authors provide their unique perspective on mass spectrometry applications that address the analysis of oil and gas, geochronology, and hydrocarbon processing. The section concludes with a chapter on the current status and prospects for renewable energy. Mass spectrometry methods have made significant contributions to archaeology. Section X focuses on recent work to give the reader historical and background information as well as specific studies that require careful field work (collection of the actual samples!) along with trace analysis using mass spectrometry-based methods. Surface analysis is a challenging area of study with very specific criteria for analysis. Section XI provides perspective and recent methods in the area of semiconductor research, organic film analysis, and characterization of ceramic materials. Section XII provides perspective on the role and uses of mass spectrometry in polymer research. Background and methodology are highlighted from three leading laboratories. Specialized analytical techniques are presented in Section XIII. The section begins with a chapter on the approaches used for the measurement of metals and alloys followed by a variety

of interesting techniques that involve the use of thin layer chromatography, laser ionization, steady-state isotopic transient kinetic analysis, and proton transfer reaction mass spectrometry.

It is my sincere hope that the handbook provides the information and details to assist scientists with current work as well as inspire future studies. Also, because of the vast content of work, it is hoped that seemingly unrelated applications provide helpful insight into novel uses of mass spectrometry and promote new areas of research.

Finally, I wish to acknowledge the contributions of many—authors, collaborators, editors, and families—

who made this handbook possible. Also, along with the terrific editorial staff at John Wiley & Sons, I would like to give a special acknowledgment to Gladys Mok, Managing Editor at John Wiley & Sons, for her significant contributions and premier support during this project.

MIKE S. LEE

*Milestone Development Services
August 2011*

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