

PREFACE

Mass spectrometry is a rapidly changing field of science that has experienced substantial development of new instrumentation along with increased applications in the area of biomolecule analysis. This book is addressing these new aspects by presenting the latest developed mass spectrometers and ionization techniques. The greater majority of mass spectral analysis of biomolecules in the laboratory today use ionization sources that produce even electron ions as opposed to odd electron ion spectra. Traditionally, mass spectral interpretation books have focused solely on the treatment of odd electron spectra generated from electron ionization (EI) sources. While electron ionization is still used to some extent, the majority of ionization techniques used in today's mass spectrometers incorporate sources that generate even electron ions. Furthermore, techniques such as electrospray ionization and matrix-assisted laser desorption ionization are soft ionization techniques that produce primarily intact ions as opposed to the EI source where the molecular ion is often depleted and not observed spectrally. Even electron ions give a mass-to-charge ratio (m/z , molecular weight plus weight of adduct divided by the charge) of the biomolecule being analyzed, which is often subjected to collision-induced dissociation to produce an even electron product ion spectrum that is used for structural elucidation and unknown identification.

The book is also a combination of the detailed step-by-step methodology for mass spectral interpretation that is coupled to a complete coverage of mass spectrometry and the fundamentals that underlie this extremely useful but complex subject. For the interested researcher or student, mass spectrometers are complicated instrumentation and the field of the application of mass spectrometry to biomolecule analysis is broad, complex, and can be intimidating. The book fills a need for a comprehensive understanding of mass spectrometry in conjunction with an easily understandable methodology for spectra interpretation and structural elucidation. While the book

does give a complete basic coverage of odd electron spectral interpretation, which is the focus of most mass spectrometry books used in classroom study (see Chapter 5), its main focus is upon even electron ion mass spectral interpretation. The book can be used in mass spectrometry classes giving the students a more up-to-date application of mass spectrometry. It can also be used by individuals who have had the traditional classroom introduction to mass spectrometry but who are interested in reviewing the subject and applying the technique of mass spectrometry to biomolecule analysis, which is now one of the major applications of mass spectrometry in research and industry. Upon reading and understanding this book, one can easily apply what is learned to the mass spectrometric analysis of daily routine work and to high-level research interpretation.

An introduction to mass spectrometry in conjunction with pertinent fundamentals to lay a foundation in which to build upon in later chapters is presented in Chapter 1. Chapter 2 discusses ionization techniques and sources including electron ionization and the more current soft ionization techniques of electrospray ionization and matrix-assisted laser desorption ionization at a fundamental level for an in-depth and comprehensive understanding of the ionization methods used in mass spectrometry. Chapter 3 covers the basics of the most commonly encountered mass analyzers geared toward a fundamental course in mass analyzer theory at either the undergraduate or graduate level. Gas-phase reaction rate theory and collision theory are covered in Chapter 4 to give a basic understanding behind gas-phase unimolecular reactions such as collision-induced dissociation (CID) that produce product ion spectra. A main focus of the book is presented in Chapters 5 and 6 to teach how to analyze mass spectra for unknown structure elucidation and identification. The approach presented uses techniques such as initial discussion of sample origin and spectra origination, the application of reasonable fragmentation pathways, and product ion structures. The teaching approach is to take structures of known compounds and break them apart into their basic building blocks in a kind of "exploded" representation and then relate this to a product ion spectrum by matching reasonable structures to the masses of the product ions produced in the collision-induced dissociation experiments. The following chapters are devoted to areas of biomolecule analysis by mass spectrometry including the analysis of proteins (Chapter 7), small-molecule analysis (Chapter 8), biopolymers (Chapter 9), and finally a detailed look at the postsorce decay MALDI TOF/MS analysis of phosphorylated lipids including spectral interpretation (Chapter 10).

ACKNOWLEDGMENTS

I would like to acknowledge all those whose input, review, and criticism helped enormously in the early structuring and final content of this book. I would like to include in the acknowledgment my graduate advisor Dr. Richard B. Cole where in his mass spectrometry group at the University of New Orleans the idea of this book first came to me. Also included is Dr. Jean T. Jacobs at the Louisiana State University Health Sciences Center whose biological research models, which I worked on, helped

