

BIOCHEMICAL APPLICATIONS OF MASS SPECTROMETRY

Edited by

GEORGE R. WALLER

*Department of Biochemistry
Agricultural Experiment Station
Oklahoma State University,
Stillwater, Oklahoma*

WILEY-INTERSCIENCE

**a Division of John Wiley & Sons, Inc.
New York · London · Sydney · Toronto**

CONTENTS

Introduction, by *George R. Waller*

1 A Historical Survey of Mass Spectrometry 1

- A. Applications of Stable Isotopes to the Study of Intermediary Metabolism: Historical Survey, by *Sarah Ratner*, 1
- B. Some Early Examples of the Application of Mass Spectrometry to the Elucidation of the Structure of Complex Molecules of Biological Origin, by *Einar Stenhagen*, 11

SECTION I: INSTRUMENTATION 21

2 Mass Spectrometry Instrumentation, by *J. Throck Watson*, 23

3 Mass Spectrometer Data Acquisition and Processing Systems, 51

- A. Introduction, by *George R. Waller*, 51
- B. Low-Resolution Mass Spectrometers, 52
 - 1. Michigan State University, by *Charles C. Sweeley, Bruce D., Ray, Micah I. Krichevsky, and John F. Holland*, 52
 - 2. The Upjohn Company, by *D. A. Griffith*, 58
 - 3. Washington University (St. Louis), by *W. F. Holmes*, 60
- C. High-Resolution Mass Spectrometers, 61
 - 1. Battelle Memorial Institute, by *Rodger L. Foltz, James G. Watt, and Maynard B. Neher*, 61
 - 2. Florida State University, by *Ralph C. Dougherty*, 65
 - 3. Research Triangle Institute, by *David Rosenthal*, 67
 - 4. The Upjohn Company, by *D. A. Griffith*, 68
 - 5. Yale University, by *W. J. McMurray*, 70
- D. Both High- and Low-Resolution Mass Spectrometers, 75
 - 1. Baylor College of Medicine, by *Dominic M. Desiderio, Jr., and Richard N. Stillwell*, 75
 - 2. Jet Propulsion Laboratory (California Institute of Technology), by *H. G. Boettger*, 79
 - 3. Cornell University, by *R. Venkataraghavan and F. W. McLafferty*, 90
 - 4. Karolinska Institutet (Sweden), by *R. Ryhage*, 93
 - 5. Massachusetts Institute of Technology, by *K. Biemann*, 96
 - 6. National Institutes of Health, by *Eli Gilbert*, 101
 - 7. Stanford University, by *Walter E. Reynolds*, 109
 - 8. University of Göteborg (Sweden), by *Sixten Abrahamsson*, 116
 - 9. University of Illinois, by *Karl-Eugen Habfast, J. Carter Cook, and Kenneth L. Rinehart, Jr.*, 121

SECTION II: INTERPRETATION OF MASS SPECTRA 133

- 4 Origin of Mass Spectra**, by *A. G. Harrison and C. W. Tsang*, 135
- 5 Metastable Ions as an Aid in the Interpretation of Mass Spectra**, by *J. H. Beynon and Richard M. Caprioli*, 157
- 6 Compound Identification by Computer Matching Mass Spectra**, by *R. G. Ridley*, 177
- 7 Use of a Computer to Identify Unknown Compounds: The Automation of Scientific Inference**, by *Joshua Lederberg*, 193

SECTION III: APPLICATIONS 209

- 8 Fatty Acids, by *Göran Odham and Einar Stenhagen*, 211
- 9 Complex Lipids, by *Göran Odham and Einar Stenhagen*, 229
- 10 Steroids, by *H. Budzikiewicz*, 251
- 11 Bile Acids, by *William H. Elliott*, 291
- 12 Carbohydrates, by *T. Radford and D. C. DeJongh*, 313
- 13 Terpenes and Terpenoids, by *C. R. Enzell, R. A. Appleton, and I. Wahlberg*, 351
- 14 Amino Acids, by *W. Vetter*, 387
- 15 Amino Acid Sequence in Oligopeptides, by *K. Biemann*, 405
- 16 Nucleic Acids and Derivatives, by *Charles Hignite*, 429
- 17 Antibiotics, by *Kenneth L. Rinehart, Jr., and George E. Van Lear*, 449
- 18 Vitamins and Cofactors, by *William H. Elliott and George R. Waller*, 499
- 19 Hormones, by *Lewis L. Engel and James C. Orr*, 537
- 20 Drug Metabolism, by *M. F. Grostic*, 573
- 21 Tetrapyrroles, by *Ralph C. Dougherty*, 591
- 22 Clinical Uses of Mass Spectrometry, by *K. Muysers and U. Smidt*, 601
- 23 Pesticides, by *J. N. Damico*, 623
- 24 Alkaloids, by *S. D. Sastry*, 655
- 25 Flavor Components, by *Michael G. Kolor*, 701
- 26 Semiochemicals, by *F. E. Regnier*, 723
- 27 Use of Stable Isotopes, by *Richard M. Caprioli*, 735
- 28 Negative Ions, by *Charles E. Melton*, 777
- 29 Use of Mass Spectrometry in the Detection of Life on Other Planets, by *H. G. Boettger*, 789
- 30 Determination of the Structures of Organic Molecules and Quantitative Analyses with the Field Ionization Mass Spectrometer, by *H. D. Beckey*, 795
- 31 Chemical Ionization Mass Spectrometry, by *G. P. Arsenault*, 817

SECTION IV: APPENDICES 833

- Appendix I Mass Spectrometry Data Centre (Aldermaston), by *R. G. Ridley*, 835
- Appendix II The NIH Regional Biomedical Mass Spectrometry Resources Program, by *M. Oxman*, 837
- Appendix III Mass Spectral Computer Program Exchange, by *Mynard C. Hamming*, 841
- Appendix IV List of Mass Spectrometer Manufacturers and Their Models, by *George R. Waller*, 843

Index 853