

CONTENTS

Preface

xi

Contributors

xv

1 Cultural, Serological, and Genetic Methods for Identification of Bacteria

1

John B. Sutherland and Fatemeh Rafii

- 1.1 Introduction, 1
- 1.2 Identification of Bacteria by Cultural Methods, 3
- 1.3 Identification of Bacteria by Serological Methods, 6
- 1.4 Identification of Bacteria by Genetic Methods, 8
- 1.5 Other Methods Used for Bacterial Characterization, 12
- 1.6 Conclusions, 13
- Acknowledgments, 13
- References, 13

2 Mass Spectrometry: Identification and Biodection, Lessons Learned and Future Developments

23

Alvin Fox

- 2.1 Introduction, 23
- 2.2 Analysis of Fatty Acid and Sugar Monomers by GC-FID, GC-MS, and GC-MS-MS, 24
- 2.3 Analysis of PCR Products by PCR, PCR-MS, and PCR-MS-MS, 26

- 2.4 Analysis of Proteins by MALDI-TOF MS, 31
- 2.5 Chemical Markers for Protein-Based Identification or Biodetection, 32
- 2.6 Conclusions, 33
- References, 34

3 An Introduction to MALDI-TOF MS

39

Rohana Liyanage and Jackson O. Lay, Jr.

- 3.1 Introduction, 39
- 3.2 Mass Spectrometry and Time-of-Flight MS, 40
- 3.3 Matrix-Assisted Laser Desorption Ionization, 47
- 3.4 MALDI-TOF Mass Spectrometry, 51
- 3.5 MALDI-TOF and Bacterial Identification, 51
- 3.6 Conclusions, 55
- References, 56

4 The Development of the Block II Chemical Biological Mass Spectrometer

61

Wayne H. Griest and Stephen A. Lammert

- 4.1 Introduction, 61
- 4.2 Development History and Design Philosophy, 63
- 4.3 Requirements and Specifications, 73
- 4.4 Performance Testing, 79
- 4.5 Conclusions, 86
- Acknowledgments, 87
- References, 87

5 Method Reproducibility and Spectral Library Assembly for Rapid Bacterial Characterization by Metastable Atom Bombardment Pyrolysis Mass Spectrometry

91

Jon G. Wilkes, Gary Miertschin, Todd Eschler, Les Hosey, Fatemeh Rafii, Larry Rushing, Dan A. Buzatu, and Michel J. Bertrand

- 5.1 Introduction, 91
- 5.2 Sample Preparation for Rapid, Reproducible Cell Culture, 95
- 5.3 Analytical Instrumentation for Sensitive Detection and Spectral Reproducibility, 103
- 5.4 Spectral Library Assembly, 108
- 5.5 Pattern Recognition Methods for Objectively Classifying Bacteria, 111
- 5.6 Conclusions, 120
- Acknowledgment, 121
- References, 121

6 MALDI-TOF Mass Spectrometry of Intact Bacteria	125
<i>Jackson O. Lay, Jr., and Rohana Liyanage</i>	
6.1 Introduction,	125
6.2 MALDI MS of Cellular Extracts,	127
6.3 Taxonomy: From Isolates to Whole-Cell MALDI,	129
6.4 Whole-Cell MALDI MS,	131
6.5 Biology-Based Changes in Whole-Cell MALDI Spectra,	133
6.6 Analysis of Mixtures,	134
6.7 Experimental Approaches,	136
6.8 Identification of Protein Markers,	141
6.9 Detection of Target Proteins,	142
6.10 Analysis of Clinical Isolates,	143
6.11 Conclusions,	147
References,	147
7 Development of Spectral Pattern-Matching Approaches to Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry for Bacterial Identification	153
<i>Kristin H. Jarman and Karen L. Wahl</i>	
7.1 Introduction,	153
7.2 MALDI MS Signature Library Construction and Identification,	154
7.3 Full Spectrum Pattern Methods,	155
7.4 Peak Table Based Methods,	156
7.5 Future Directions,	158
References,	159
8 Studies of Malaria by Mass Spectrometry	161
<i>Plamen A. Demirev</i>	
8.1 Introduction,	161
8.2 <i>Plasmodium</i> in Red Blood Cells,	163
8.3 Experimental Protocols for LDMS Detection of Malaria,	164
8.4 Malaria Detection by Laser Desorption Mass Spectrometry,	167
8.5 MS-Based Proteomics of the <i>Plasmodium</i> Parasite,	174
8.6 Conclusions,	175
Acknowledgments,	176
References,	176
9 Bacterial Strain Differentiation by Mass Spectrometry	181
<i>Randy J. Arnold, Jonathan A. Karty, and James P. Reilly</i>	
9.1 Introduction,	181
9.2 Analysis of Cellular Proteins by Mass Spectrometry,	182

9.3	Application of MALDI-TOF to Bacteria Identification, 183	
9.4	Conclusions, 197	
	Acknowledgment, 197	
	References, 197	
10	Bacterial Protein Biomarker Discovery: A Focused Approach to Developing Molecular-Based Identification Systems	203
	<i>Tracie L. Williams, Steven R. Monday, and Steven M. Musser</i>	
10.1	Introduction, 203	
10.2	Protein Extraction Methods, 206	
10.3	Protein Chromatography, 206	
10.4	Mass Spectrometry, 210	
10.5	Automating the Process, 212	
10.6	Collecting and Sequencing Proteins, 216	
10.7	Conclusions, 222	
	References, 222	
11	High-Throughput Microbial Characterizations Using Electrospray Ionization Mass Spectrometry and Its Role in Functional Genomics	229
	<i>Seetharaman Vaidyanathan and Royston Goodacre</i>	
11.1	Introduction, 229	
11.2	Microbial Characterizations beyond the Genomic Level: Functional Genomics, 230	
11.3	Electrospray (Ionization) Mass Spectrometry (ESMS), 233	
11.4	ESMS of Microbes, 237	
11.5	Direct Infusion ESMS of Crude Cell extracts for High-Throughput Characterizations—Metabolic Fingerprinting and Footprinting, 247	
11.6	Conclusions, 249	
	Acknowledgment, 250	
	References, 250	
12	Bioinformatics for Flexibility, Reliability, and Mixture Analysis of Intact Microorganisms	257
	<i>Catherine Fenselau and Patrick Pribil</i>	
12.1	Introduction, 257	
12.2	Library Matching, 259	
12.3	Machine Learning, 259	
12.4	Bioinformatics, 259	
12.5	Protein Molecular Masses, 262	
12.6	Peptide Maps, 265	

12.7	Microsequences from Peptides and Proteins, 265	
12.8	Remaining Challenges, 269	
12.9	Conclusions, 270	
	Acknowledgments, 270	
	References, 270	
13	MALDI-FTMS of Whole-Cell Bacteria	279
	<i>Jeffrey J. Jones, Michael J. Stump, and Charles L. Wilkins</i>	
13.1	Introduction, 279	
13.2	Fundamentals of MALDI-FTMS, 280	
13.3	Fundamentals of Complex Biological Analysis, 282	
13.4	Whole-Cell Characterization through MALDI-FTMS, 283	
13.5	Recombinant Overexpressed Proteins Desorbed Directly from Whole Cells, 293	
13.6	Conclusions, 295	
	References, 296	
14	A Review of Antibody Capture and Bacteriophage Amplification in Connection with the Direct Analysis of Whole-Cell Bacteria by MALDI-TOF-MS	301
	<i>Kent J. Voorhees and Jon C. Rees</i>	
14.1	Introduction, 301	
14.2	Bacterial Identification, 303	
14.3	Immunocapture of Bacterial Mixtures, 308	
14.4	Bacteriophage Amplification of Bacteria, 311	
14.5	Conclusions, 315	
	References, 316	
15	Discrimination and Identification of Microorganisms by Pyrolysis Mass Spectrometry: From Burning Ambitions to Cooling Embers—A Historical Perspective	319
	<i>Éadaoin Timmins and Royston Goodacre</i>	
15.1	Introduction to Microbial Characterization, 319	
15.2	Principles of PyMS, 323	
15.3	Early Developments and Investigations, 1952 to 1985, 325	
15.4	The mid-1980s and Beyond, 327	
15.5	The Move from Cluster Analyses to Neural Networks, 330	
15.6	Reproducibility of PyMS, 332	
	Acknowledgment, 334	
	References, 334	
	Index	345