
TABLE OF CONTENTS

The Editor	xiii
The Contributors	xv
The Sponsors	xix
Foreword	xxiii
Introduction	xxvii
Chapter 1 General Principles of Mass Spectrometry	1
<i>Albert T. Lebedev</i>	
1.1 Basic concepts	1
1.2 Sample introduction	3
1.3 Ionisation	5
1.4 Mass analysers	11
1.5 Detection of ions	18
References	19
Chapter 2 Gas Chromatography/Mass Spectrometry: A Workhorse of Modern Environmental Analysis	21
<i>Albert T. Lebedev</i>	
2.1 General aspects	21
2.2 Types of chromatograms based on ion current	22
2.3 Acquisition rate	32
2.4 Compounds amenable to GC/MS	33
2.5 Quantitative analysis	35
2.6 Conclusions	40
References	40
Chapter 3 Liquid Chromatography/Mass Spectrometry: The Method of Choice for the Qualitative and Quantitative Analysis of Environmental Pollutants	41
<i>G�rard Bondoux and Jean-Marc Joumier</i>	
3.1 Introduction	41
3.2 Techniques and instruments of interest for environmental analysis	42
3.3 Coupling an LC to an MS: the challenges and the solutions	43
3.4 API	45
3.5 Types of mass spectrometers and their capabilities for environmental analysis	47

3.6	Measuring real samples	52
3.7	Main applications of interest	52
3.8	Confirmatory analysis	53
3.9	Targeted approaches using tandem quadrupole instruments	54
3.10	Screening and investigative methods using a QTOF instrument	59
3.11	Why use a QTOF for environmental analysis?	60
3.12	Research work on transformation products	64
3.13	Short- and medium-term perspectives	64
	References	65
Chapter 4	Mass Spectrometry/Mass Spectrometry Approaches for the Analysis of Environmental Pollutants	67
	<i>Don Betowski</i>	
4.1	Introduction	67
4.2	Mass spectrometry/mass spectrometry instrumentation	68
4.3	Environmental applications of MS/MS	73
4.4	Summary	83
4.5	Notice	83
	References	84
Chapter 5	Informatics and Mass Spectral Databases in the Evaluation of Environmental Mass Spectral Data	89
	<i>O. David Sparkman</i>	
5.1	Introduction	89
5.2	Mass spectral databases and database search programs	92
5.3	Evolution of mass spectral databases	93
5.4	Mass spectral databases	95
5.5	Other mass spectral databases	96
5.6	Caution about data acquisition when planning to use database searches	98
5.7	Mass spectral database search programs (software that searches the database)	98
5.8	Example showing Agilent PBM search giving the clearest answer	99
5.9	Example showing NIST MS search giving the clearest answer	104
5.10	Which search algorithm is the best?	106
5.11	NIST MS Interpreter	106
5.12	Using the NIST EI mass spectral database with liquid chromatography/mass spectrometry data	109
5.13	NIST Retention Index Database	111
5.14	Automated mass spectral deconvolution and identification system (AMDIS) from NIST	112
5.15	Accurate mass measurements for the masses	116
5.16	Other software of interest to the environmental mass spectrometrists	117
5.17	Concluding remarks	120
	References	120

Chapter 6	Advanced Gas Chromatography/Mass Spectrometry Methods	123
	<i>Konstantin A. Artemenko, Alexander B. Fialkov, Alexander Gordin, Aviv Amirav and Albert T. Lebedev</i>	
6.1	Fast gas chromatography/mass spectrometry mode	123
6.2	GC/MS with supersonic molecular beams interface	130
6.3	Comprehensive two-dimensional GC/GC/MS technology	138
6.4	Concluding remarks	145
	References	145
Chapter 7	Ambient Mass Spectrometry: Environmental Analysis Without Sample Preparation	147
	<i>Rosana M. Alberici, Rosineide C. Simas and Marcos N. Eberlin</i>	
7.1	Introduction	147
7.2	Major ambient mass spectrometry techniques	148
7.3	Environmental applications	155
7.4	Conclusions	159
	References	162
Chapter 8	Desorption Electrospray Ionisation Mass Spectrometry	167
	<i>Zoltán Takáts</i>	
8.1	Introduction	167
8.2	Experimental set-up and conditions	168
8.3	Reactive desorption	170
8.4	Mass spectrometric imaging by DESI	172
8.5	Quantitative determinations	174
8.6	Water analysis	175
8.7	Aerosol analysis	177
8.8	Direct analysis	180
8.9	Future directions	181
	References	181
Chapter 9	Miniaturised Mass Spectrometers for Environmental Analysis	185
	<i>Gautam Sharma, Robert J. Noll, Zheng Ouyang and R. Graham Cooks</i>	
9.1	Introduction	185
9.2	Fundamentals of the instrumentation	187
9.3	Environmental applications of miniature mass spectrometry	204
9.4	Summary	218
	References	218
Chapter 10	Inductively Coupled Plasma Mass Spectrometry in Environmental Analysis	225
	<i>Alexey Leykin and Simon Nelms</i>	
10.1	Introduction	225
10.2	Basic principles	226
10.3	Benefits and challenges	227
10.4	Applications	229
	References	235

Chapter 11 Mass Spectrometry's Role in Studies of Volatile Organic Pollutants	239
<i>Simin D. Maleknia</i>	
11.1 Introduction to volatile organic pollutants	239
11.2 Mass spectrometry methods for the analysis of volatile pollutants	241
11.3 Monitoring pollutants from ambient to wildfire conditions	246
11.4 Concluding remarks and future work	254
Acknowledgements	255
References	258
Chapter 12 Mass Spectrometry Identification and Quantification of Toxicologically Important Drinking Water Disinfection By-Products	263
<i>Susan D. Richardson</i>	
12.1 Introduction	263
12.2 Analytical methods for identifying and quantifying DBPs	268
12.3 What does the future hold?	280
Acknowledgements	281
References	281
Chapter 13 Emerging Contaminants in the Environment	287
<i>Tammy L. Jones-Lepp</i>	
13.1 Introduction	287
13.2 Mass spectrometry for the analysis of emerging contaminants	289
13.3 Conclusions	301
Acknowledgements	301
Note	303
References	303
Chapter 14 Pesticide Residue Analysis in Environmental Samples by Hyphenated Chromatography/Mass Spectrometry	309
<i>F. Hernández, M. Ibáñez and T. Portolés</i>	
14.1 Introduction	309
14.2 Pesticides residue analysis	310
14.3 GC/MS analysis	313
14.4 LC/MS analysis	316
14.5 Trends	322
Acknowledgements	326
References	326
Chapter 15 Analysis of Persistent Halogenated Compounds: Chlorinated Dibenzo-<i>p</i>-dioxins and Dibenzofurans	329
<i>Ray Clement and Eric J. Reiner</i>	
15.1 Introduction	329
15.2 Sample preparation for trace analysis of CDDs/CDFs	332
15.3 Quantitative analysis and the use of isotope dilution techniques	336
15.4 GC methods	339
15.5 Mass spectrometric methods	340
15.6 Complete analytical methods for CDDs/CDFs and other persistent halogenated compounds	345

15.7 The future of multi-residue methods	345
References	349
Chapter 16 Mass Spectrometry of Atmospheric Aerosols	353
<i>Klaus-Peter Hinz</i>	
16.1 Introduction	353
16.2 Aerosol properties and effects	353
16.3 Instrumentation and applications	357
16.4 Summary and future outlook	379
References	381
Chapter 17 Mass Spectrometry in the Study of Interactions of Environmental Pollutants with DNA	387
<i>Natalia Tretyakova and Melissa Goggin</i>	
17.1 Introduction	387
17.2 Sources of DNA for adduct analyses	388
17.3 Sample preparation	390
17.4 MS instrumentation for HPLC/ESI ⁺ -MS/MS of DNA adducts	390
17.5 Examples of HPLC/ESI-MS/MS analyses of DNA adducts	393
17.6 New approaches to improve analytical methods for DNA adduct analysis	402
17.7 Conclusions	407
Acknowledgements	408
References	408
Chapter 18 Petroleomics and the Analysis of Complex Organic Mixtures with Fourier Transform Ion Cyclotron Resonance	415
<i>Vladislav V. Lobodin, Ryan P. Rodgers and Alan G. Marshall</i>	
18.1 Introduction	415
18.2 FT-ICR MS	416
18.3 Mass resolution, mass resolving power and mass accuracy	420
18.4 Exact mass and mass defect	423
18.5 Double bond equivalents and the Z number	426
18.6 Kendrick mass and Kendrick mass defect	427
18.7 Data visualisation: Kendrick plot, van Krevelen diagram, class distribution, DBE versus carbon number plot	428
18.8 Ionisation methods for complex mixture analysis by FT-ICR MS	433
18.9 Application of FT-ICR to environmental problems	435
References	439
Chapter 19 Ultrahigh Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for the Analysis of Natural Organic Matter from Various Environmental Systems	443
<i>Ph. Schmitt-Kopplin, M. Harir, D. Tziotis, Z. Gabelica and N. Hertkorn</i>	
19.1 Introduction	443
19.2 Materials and methods	447
19.3 Results and discussion	448

19.4	Conclusions	455
	References	456
Chapter 20	Mass Spectrometry Imaging	461
	<i>Bernhard Spengler</i>	
20.1	Introduction	461
20.2	Microprobes and molecular imaging	461
20.3	Visualising spatial and compositional information	462
20.4	The matrix problem	465
20.5	SIMS imaging: entering bioanalytics	466
20.6	Imaging quality and intrinsic LOD	467
20.7	MS imaging as a qualitative method	468
20.8	MS imaging as an exact analytical method	469
20.9	Identification and characterisation	469
20.10	MS imaging in environmental sciences	471
20.11	Outlook	471
	References	474
Chapter 21	Isotope Ratio Mass Spectrometry	475
	<i>Anzhelika Talibova, Michael Tokarev and Andreas Hilkert</i>	
21.1	Introduction	475
21.2	The delta value	475
21.3	Causes of the variations of stable isotopes in nature	476
21.4	Gas isotope ratio mass spectrometry	478
21.5	Sample preparation devices and interfaces	480
21.6	Some applications	485
	References	490
Index		491