

CONTENTS

Contributors	ix
Preface	xi
1 Introduction	1
<i>Luigi Mondello, Peter Q. Tranchida, and Keith D. Bartle</i>	
1.1 Two-Dimensional Chromatography–Mass Spectrometry: A 50-Year-Old Combination, 2	
1.2 Shortcomings of One-Dimensional Chromatography, 3	
1.3 Benefits of Two-Dimensional Chromatography, 6	
1.4 Book Content, 7	
1.5 Final Considerations, 11	
2 Multidimensional Gas Chromatography: Theoretical Considerations	13
<i>Leonid M. Blumberg</i>	
2.1 Symbols, 15	
2.2 One-Dimensional GC, 17	
2.3 Comprehensive GC × GC, 31	
3 Multidimensional Liquid Chromatography: Theoretical Considerations	65
<i>Pavel Jandera</i>	
3.1 Two-Dimensional LC Techniques, 66	

- 3.2 Peak Capacity in HPLC: One- and Multidimensional Separations, 69
 - 3.3 Orthogonality in Two-Dimensional LC–LC Systems, 73
 - 3.4 Sample Dimensionality and Structural Correlations, 75
 - 3.5 Separation Selectivity and Selection of Phase Systems in Two-Dimensional LC–LC, 79
 - 3.6 Programmed Elution in Two-Dimensional HPLC, 81
 - 3.7 Fraction Transfer Modulation in Comprehensive LC \times LC: Additional Band Broadening, 87
 - 3.8 Future Perspectives, 89
- 4 History, Evolution, and Optimization Aspects of Comprehensive Two-Dimensional Gas Chromatography 93**
- Ahmed Mostafa, Tadeusz Górecki, Peter Q. Tranchida, and Luigi Mondello*
- 4.1 Fundamentals of GC \times GC, 94
 - 4.2 Modulation, 96
 - 4.3 GC \times GC Data Interpretation, 97
 - 4.4 GC \times GC Instrumentation, 100
 - 4.5 Thermal Modulators, 101
 - 4.6 Comprehensive Two-Dimensional GC Method Optimization, 115
 - 4.7 Final Remarks, 140
- 5 Flow-Modulated Comprehensive Two-Dimensional Gas Chromatography 145**
- John V. Seeley*
- 5.1 Timing Requirements of GC \times GC Modulators, 145
 - 5.2 Criteria for Evaluating Modulators, 150
 - 5.3 Forms of Modulation, 151
 - 5.4 Single-Stage Flow Modulation, 152
 - 5.5 Two-Stage Flow Modulation, 157
 - 5.6 Summary of Flow Modulators, 167
 - 5.7 Brief Comparison to Thermal Modulation, 169
 - 5.8 Concluding Remarks, 169
- 6 Comprehensive Two-Dimensional Gas Chromatography Combined with Mass Spectrometry 171**
- Peter Q. Tranchida, Luigi Mondello, Samuel D. H. Poynter, and Robert A. Shellie*
- 6.1 Instrument Requirements for GC \times GC–MS, 173
 - 6.2 Data Processing of GC \times GC–TOF MS Results, 180
 - 6.3 Method Translation in GC \times GC–MS, 181
 - 6.4 GC \times MS, 181

- 6.5 Conventional and Alternative Modulation Techniques for GC \times GC-MS, 184
- 6.6 GC \times GC-MS Applications, 187
- 6.7 Concluding Remarks, 232
- 7 Detector Technologies and Applications in Comprehensive Two-Dimensional Gas Chromatography 243**
Philip J. Marriott
- 7.1 Detection in GC \times GC, 244
- 7.2 Comments on GC \times GC with Mass Spectrometry, 249
- 7.3 Flame Ionization Detection in GC \times GC, 250
- 7.4 Electron Capture Detection in GC \times GC, 254
- 7.5 Sulfur Chemiluminescence Detection in GC \times GC, 260
- 7.6 Nitrogen Chemiluminescence Detection in GC \times GC, 263
- 7.7 Atomic Emission Detection in GC \times GC, 265
- 7.8 Thermionic Detection in GC \times GC, 267
- 7.9 Flame Photometric Detection in GC \times GC, 269
- 7.10 Case Study of GC \times GC with Selective Detection, 272
- 7.11 Dual Detection with GC \times GC, 274
- 7.12 Conclusions, 275
- 8 History, Evolution, and Optimization Aspects of Comprehensive Two-Dimensional Liquid Chromatography 281**
Isabelle François, Koen Sandra, and Pat Sandra
- 8.1 Method Development and Instrumentation, 282
- 8.2 Technical Problems in Comprehensive Liquid Chromatography, 309
- 8.3 Detection, 314
- 8.4 Data Representation, 315
- 8.5 Instrumentation, 316
- 8.6 Milestones in Comprehensive Liquid Chromatography, 317
- 8.7 Applications, 320
- 8.8 Beyond Two-Dimensional Chromatography, 320
- 8.9 Comparison of LC \times LC and Off-Line 2D LC, 321
- 8.10 Conclusions, 325
- 9 Comprehensive Two-Dimensional Liquid Chromatography Combined with Mass Spectrometry 331**
Paola Dugo, Luigi Mondello, Francesco Cacciola, and Paola Donato
- 9.1 HPLC-MS, 332
- 9.2 LC \times LC-MS Instrumentation and Method Development, 334
- 9.3 LC \times LC-MS Applications, 336

10	Comprehensive Two-Dimensional Liquid Chromatography Applications	391
	<i>Paola Dugo, Luigi Mondello, Francesco Cacciola, and Paola Donato</i>	
10.1	Comprehensive 2D LC Separation of Synthetic and Natural Polymers, 392	
10.2	Comprehensive 2D LC Separation of Natural Products and Antioxidants, 399	
10.3	Comprehensive 2D LC Separation of Pharmaceutical and Environmental Compounds, 412	
10.4	Comprehensive 2D LC Separation of Proteins and Peptides, 417	
11	Other Comprehensive Chromatography Methods	429
	<i>Isabelle François, Pat Sandra, Danilo Sciarrone, and Luigi Mondello</i>	
11.1	Online Two-Dimensional Liquid Chromatography–Gas Chromatography, 430	
11.2	Online Two-Dimensional Supercritical Fluid Chromatography–Gas Chromatography, 440	
11.3	Online Two-Dimensional Supercritical Fluid Chromatography–Supercritical Fluid Chromatography, 440	
11.4	Online Two-Dimensional Supercritical Fluid Chromatography–Liquid Chromatography, 442	
12	Comprehensive Chromatography Data Interpretation Technologies	449
	<i>Elizabeth M. Humston and Robert E. Synovec</i>	
12.1	Higher-Order Data Structure, 450	
12.2	Modifications of First-Order Data-Handling Approaches, 453	
12.3	Visualization, 456	
12.4	Mass Spectral Detection, 461	
12.5	Chemometrics, 463	
12.6	Summary of Data Interpretation Technologies, 472	
	Index	477