
Contents

Preface..... xv
Contributors xvii

SECTION I *Method Development and Optimization*

Chapter 1 Experimental Design in Chromatographic Method Development and Validation 3
 Lukasz Komsta and Yvan Vander Heyden

Chapter 2 Chromatographic Response Functions..... 25
 Regina M.B.O. Duarte, João T.V. Matos, and Armando C. Duarte

Chapter 3 Chemometric Strategies to Characterize, Classify, and Rank Chromatographic
 Stationary Phases and Systems 45
 Charlene Muscat Galea, Debby Mangelings, and Yvan Vander Heyden

SECTION II *Univariate Analysis*

Chapter 4 Chromatographic Applications of Genetic Algorithms 63
 Mohammad Goodarzi and Yvan Vander Heyden

Chapter 5 Statistics in Validation of Quantitative Chromatographic Methods 77
 Eliangiringa Kaale, Danstan Hipolite Shewiyo, and David Jenkins

Chapter 6 Calibration Curves in Chromatography 99
 Sven Declerck, Johan Viaene, Ines Salsinha, and Yvan Vander Heyden

SECTION III *Data Preprocessing and Unsupervised Analysis*

Chapter 7 Introduction to Multivariate Data Treatment..... 117
 Lukasz Komsta and Yvan Vander Heyden

Chapter 8 Introduction to Exploratory and Clustering Techniques 127
 Ivana Stanimirova and Michał Daszykowski

Chapter 9	Denoising of Signals, Signal Enhancement, and Baseline Correction in Chromatographic Science	137
	<i>Zhi-Min Zhang, Hong-Mei Lu, and Yi-Zeng Liang</i>	
Chapter 10	Alignment of One- and Two-Dimensional Chromatographic Signals	171
	<i>Michał Daszykowski</i>	
Chapter 11	Peak Purity and Resolution of Chromatographic Data	183
	<i>Sílvia Mas and Anna de Juan</i>	
Chapter 12	Modeling of Peak Shape and Asymmetry	217
	<i>José Ramón Torres-Lapasió, Juan José Baeza-Baeza, and María Celia García-Álvarez-Coque</i>	
Chapter 13	Missing and Censored Data in Chromatography	239
	<i>Ivana Stanimirova</i>	

SECTION IV *Classification, Discrimination, and Calibration*

Chapter 14	Linear Supervised Techniques.....	255
	<i>Łukasz Komsta and Yvan Vander Heyden</i>	
Chapter 15	Discriminant Analysis and Classification of Chromatographic Data.....	267
	<i>Alessandra Biancolillo and Federico Marini</i>	
Chapter 16	Nonlinear Supervised Techniques	285
	<i>Geert Postma, Lionel Blanchet, Frederik-Jan van Schooten, and Lutgarde Buydens</i>	

SECTION V *Retention Modeling*

Chapter 17	Introduction to Quantitative Structure–Retention Relationships	303
	<i>Krzyszimir Ciura, Piotr Kawczak, Joanna Nowakowska, and Tomasz Bączek</i>	
Chapter 18	Topological Indices in Modeling of Chromatographic Retention.....	319
	<i>Małgorzata Dołowy, Katarzyna Bober, and Alina Pyka-Pająk</i>	

SECTION VI *Application Overviews*

Chapter 19 Introduction to Herbal Fingerprinting by Chromatography 351
Johan Viaene and Yvan Vander Heyden

Chapter 20 Chemometric Strategies in Analysis of Chromatographic–Mass Spectrometry
Data 371
Samantha Riccadonna and Pietro Franceschi

Chapter 21 Chemometric Strategies in Chromatographic Analysis of Pharmaceuticals 381
Erdal Dinç

SECTION VII *Miscellaneous*

Chapter 22 Bayesian Methods in Chromatographic Science..... 417
David Brynn Hibbert

Chapter 23 Multiway Methods in Chromatography 435
Lukasz Komsta and Yvan Vander Heyden

Chapter 24 Recurrent Relationships in Separation Science..... 449
Igor Zenkevich

Chapter 25 Chemometrics and Image Processing in Thin-Layer Chromatography 469
*Bahram Hemmateenejad, Elaheh Talebanpour Bayat, Elmira Rafatmah,
Zahra Shojaeifard, Nabiollah Mobaraki, and Saeed Yousefinejad*

Index..... 495