## **Contents**

	List of Abbreviations $VII$ Symbols $IX$
1	What is Chemometrics? 1
1.1	The Computer-Based Laboratory 2
1.2	Statistics and Data Interpretation 10
1.3	Computer-Based Information Systems/Artificial
	Intelligence 11
	General Reading 12
	Questions and Problems 13
2	Basic Statistics 15
2.1	Descriptive Statistics 16
2.2	Statisticai Tests 28
2.3	Analysis of Variance 44
	General Reading 50
	Questions and Problems 52
3	Signal Processing and Time Series Analysis 55
3.1	Signal Processing 56
3.2	Time Series Analysis 83
	General Reading 90
	Questions and Problems 91
4	Optimization and Experimental Design 93
4.1	Systematic Optimization 94
4.2	Objective Functions and Factors 95
4.3	Experimental Design and Response Surface
	Methods 102
4.4	Sequential Optimization: Simplex Method 125
	General Reading 132
	Ouestions and Problems 133

VI [	Contents	
·	5	Pattern Recognition and Classification 135
	5.1	Preprocessing of Data 137
	5.2	Unsupervised Methods 140
	5.3	Supervised Methods 184
		General Reading 209
		Questions and Problems 210
	6	Modeling 213
	6.1	Univariate Linear Regression 214
	6.2	Multiple Linear Regression 231
	6.3	Nonlinear Methods 258
		General Reading 269
		Questions and Problems 271
	7	Analytical Databases 273
	7.1	Representation of Analytical Information 274
	7.2	Library Search 286
	7.3	Simulation of Spectra 292
		General Reading 294
		Questions and Problems 295
	8	Knowledge Processing and Soft Computing 297
	8.1	Artificial Intelligence and Expert Systems 297
	8.2	Neural Networks 306
	8.3	Fuzzy Theory, 321
	8.4	Genetic Algorithms and Other Global Search
		Strategies 334
		General Reading 342
		Questions and Problems 344
	9	Quality Assurance and Good Laboratory Practice 345
	9.1	Validation and Quality Control 346
	9.2	Accreditation and Good Laboratory Practice 351
		General Reading 352
		Questions and Problems 353
		Appendix 355

Index 371