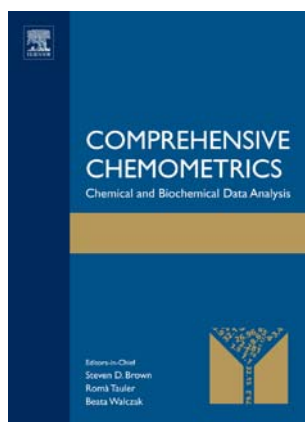


# Steven D. Brown, Romà Tauler, Beata Walczak (Eds.): Comprehensive chemometrics. Chemical and biochemical data analysis

Jürgen W. Einax

© Springer-Verlag 2009



## Bibliography

Comprehensive chemometrics.  
Chemical and biochemical data  
analysis  
Steven D. Brown, Romà Tauler,  
Beata Walczak (Eds.)  
Elsevier  
ISBN: 978-0-444-52702-8  
Hardcover, 2.200 pages,  
March 2009, € 1360

**Contents** “Comprehensive Chemometrics” is, as the title promises, a comprehensive four-volume set with 12 sections and 90 individual contributions written by leading experts and integrated by a hierarchy of three editors-in-chief, ten section editors, and many authors from 21 countries. This state-of-the-art of chemometrics occupies ca 2800 pages, realized in 7.4 kg of books. The result of careful editing is a well-balanced major reference book about the current state of the entire field of chemometrics.

The first volume of the book starts with basic statistics including implementations of robust and Bayesian techniques. In subsequent chapters, methods for statistical optimization and genetic algorithms are discussed, including a section on experimental design that covers classical and non-classical methods of optimal experimental planning.

The second volume explains different methods of signal processing, for example the optimization of signal-to-noise ratio. The authors describe linear soft-modeling, focusing on novel fields of multivariate curve resolution. They complete this volume with a section on classical methods of unsupervised data mining, for example algorithms of cluster analysis.

Volume 3 contains two sections on regression analysis. First, linear regression modeling is discussed. The authors then cover selection of variables and handling of missing data. Additionally, they provide comprehensive knowledge for multivariate and multi-way regression for calibration, Kernel methods, and traditional approaches of non-linear regression. The section “Classification” is about discriminant analysis and artificial neural networks. Here, the reader learns about different approaches for feature selection, using the PLS algorithm, genetic algorithms, and wavelet transformation. Finally, volume 3 is completed by a contribution about robust multivariate techniques.

Volume 4 is dedicated to examples in chemometrics. The authors succeed in explaining complex approaches in

**Book's topic** Chemometrics has developed impressively over recent decades. New principles and methods, and many new fields of application, have appeared. The new reference book “Comprehensive Chemometrics”, available in a four-volume set (paper or online version), is an integrated account of the present state of chemical and biochemical data analysis and manipulation at a high scientific level. The work covers the main topics of chemometrics, ranging from statistics, through data acquisition and analysis, to application. This source gives the reader quick access to answers and specific information about the topics.

J. W. Einax (✉)

Institut für Anorganische und Analytische Chemie, Lehrbereich  
Umweltanalytik, Friedrich-Schiller-Universität Jena,  
Lessingstr. 8,  
07743 Jena, Germany  
e-mail: juergen.einax@uni-jena.de

chemometrics to non-experts using case studies from selected disciplines, for example environmental and food chemistry and genomics. There are also applications from the topics of image, array, and sensory data analysis. Volume 4 concludes with contributions combining chemometrics with chemoinformatics. As its final part, volume 4 contains an extensive index. Separate indices are in the individual volumes.

**Comparison with existing literature** The modern literature of chemometrics has improved in recent years. However, it is mainly dedicated exclusively to specific areas of chemometrics, for example experimental design, signal processing, and data analysis. The textbook by Massart et al. [1, 2] provides a complete overview of chemometrics, however it was published more than a decade ago. Because of the rapid development of methods in chemometrics and the growing field of application within recent years, such a reference book was needed. The new four-volume edition “Comprehensive Chemometrics” fulfills this gap and surely can serve as an ultimate and complete reference book in the field of chemometrics.

**Critical assessment** “Comprehensive chemometrics” will be a major reference book of modern chemometrics. It includes not only theoretical description of the methods and algorithms in chemometrics, but also shows the advantages and limitations of the methods described. It is characterized by many illustrative examples from real-world studies, mostly from chemistry and biochemistry. The contributions from the authors also contain advice on useful software and current references.

The excellent lay-out of the book, many tables, and informative (mostly color) figures are very helpful for easy access to the overall content.

Slight differences can be identified in the writing style in the different authors’ contributions. This leads to inconsistencies such as the use of different symbols to represent the same variable in different sections of the book. A

symbol index is missing from some contributions. However, this marginal criticism does not affect the excellent impression made by this book.

**Readership recommendation** The book covers the entire field of chemometrics and it is written at a high scientific level. It can be recommended for graduate students and researchers with a knowledge of statistics and matrix algebra who are interested in understanding the methods of chemometrics, their advantages and limitations, and their applications in chemistry and biochemistry. The integration of many practical examples, software advice, and current references give the reader fast, efficient, and solid access to classical and new methods of chemometrics.

**Summary** “Comprehensive Chemometrics” can be recommended as a new reference book to the broad range of modern chemometrics. It is written by leading experts at a high scientific level in an understandable style. A comprehensive introduction to chemometrics, the main methods, detailed reviews and illustrations, and many examples in chemistry and biochemistry, are presented in the book. The book also provides a global perspective in the rapidly evolving field of chemometrics. Overall, the book is an excellent source of up-to-date information and will be essential for researchers and others working in the field of chemometrics. The editors deserve to be congratulated for succeeding in assembling so many chapters from so many excellent contributors.

## References

1. Massart DL, Vandeginste BGM, Buydens LMC, De Jong S, Lewi PJ, Smeyers-Verbeke J (1997) Handbook of chemometrics and qualimetrics: part A. Elsevier, Amsterdam
2. Vandeginste BGM, Massart DL, Buydens LMC, De Jong S, Lewi PJ, Smeyers-Verbeke J (1998) Handbook of chemometrics and qualimetrics: part B. Elsevier, Amsterdam