

Chemometrics In Analytical Spectroscopy Rsc Rsc Analytical Spectroscopy Series

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Chemometrics in Analytical Spectroscopy 2nd Edition provides a tutorial approach to the development of chemometric techniques and their application to the interpretation of analytical spectroscopic data. From simple descriptive statistics to the more sophisticated modelling techniques of principal components analysis and partial least squares regression, this updated edition provides necessary background, enhanced by case studies. The extensive use of worked examples throughout gives Chemometrics in Analytical Spectroscopy 2nd Edition special relevance in teaching and introducing chemometrics to undergraduates and post-graduates. The book is also ideal for analysts with little specialist background. Extracts from reviews of 1st Edition: "Adams has succeeded in providing a text which is focused on analytical spectroscopy and that gently guides the reader through the concepts without recourse to too much matrix algebra." Trends in Analytical Chemistry " ... a very good introductory text for those wishing to understand the workings of chemometrics techniques." The Analyst

Chemometrics in Analytical Spectroscopy provides students and practising analysts with a tutorial guide to the use and application of the more commonly encountered techniques used in processing and interpreting analytical spectroscopic data. In detail the book covers the basic elements of univariate and multivariate data analysis, the acquisition of digital data and signal enhancement by filtering and smoothing, feature selection and extraction, pattern recognition, exploratory data analysis by clustering, and common algorithms in use for multivariate calibration techniques. An appendix is included which serves as an introduction or refresher in matrix algebra. The extensive use of worked examples throughout gives Chemometrics in Analytical Spectroscopy special relevance in teaching and introducing chemometrics to undergraduates and post-graduates undertaking analytical science courses. It assumes only a very moderate level of mathematics, making the material far more accessible than other publications on chemometrics. The book is also ideal for analysts with little specialist background in statistics or mathematical methods, who wish to appreciate the wealth of material published in chemometrics.

This practical introduction is the first to present the principles of experimental designs, optimization and multivariate regression for atomic spectroscopists.

The extensive use of worked examples throughout gives Chemometrics in Analytical Spectroscopy 2nd Edition special relevance in teaching and introducing chemometrics to undergraduates and post-graduates. The book is also ideal for analysts with little specialist background.

Covering topics including solvent selection, miniaturization and metrics for the evaluation of greenness this is a useful resource for researchers interested in reducing the risks and environmental impacts of analytical methods.

During the last two decades, the use of NMR spectroscopy for the characterization and analysis of food materials has flourished, and this trend continues to increase today. Currently, there exists no book that fulfils specifically the needs of food scientists that are interested in adding or expanding the use of NMR spectroscopy in their arsenal of food analysis techniques. Current books and monographs are rather addressed to experienced researchers in food analysis providing new information in the field. This book, written by acknowledged experts in the field, fills the gap by offering a day to day NMR guide for the food scientist, affording not only the basic theoretical aspects of NMR spectroscopy, but also practical information on sample preparation, experimental conditions and data analysis. Current developments in the field covered in this book are the availability of solid state NMR experiments such as CP/MAS and more importantly HR-MAS NMR for the analysis of semisolid foods, and the increasing use of chemometrics to analyze NMR data in food metabonomics. Moreover, this book contains an up to date discussion of MRI in food analysis including topics such as food processing and natural changes in food such as ripening. The book is a compact and complete source of information for food scientists who wish to apply methodologies based on NMR spectroscopy in food analysis. It contains information so far scattered in the primary literature, in NMR treatises and food analysis books, in a concise format that makes it appealing to food scientists who have no or minimal experience in magnetic resonance techniques. The inclusion of practical information about NMR instrumentation, experiment setup, acquisition and spectral analysis for the study of different food categories make this book a hands-on manual for food scientists wishing to implement novel NMR spectroscopy-based analytical techniques in their field.

Providing an easy explanation of the fundamentals, methods, and applications of chemometrics [] Acts as a practical guide to multivariate data analysis techniques [] Explains the methods used in Chemometrics and teaches the reader to perform all relevant calculations [] Presents the basic chemometric methods as worksheet functions in Excel [] Includes Chemometrics Add In for download which uses Microsoft Excel® for chemometrics training [] Online downloads includes workbooks with examples

This unique text blends together state estimation and chemometrics for the application of advanced data-processing techniques. State Estimation in Chemometrics, second edition describes the basic methods for chemical analysis—the multicomponent, calibration and titration systems—from a new perspective. It succinctly reviews the history of state estimation and chemometrics and provides examples of its many applications, including classical estimation, state estimation, nonlinear estimation, the multicomponent, calibration and titration systems and the Kalman filter. The concepts are introduced in a logical way and built up systematically to appeal to specialist post-graduates working in this area as well as professionals in other areas of chemistry and engineering. This new edition covers the latest research in chemometrics, appealing to readers in bio-engineering, food science, pharmacy, and the life sciences fostering cross-disciplinary research. Features a new chapter surveying the most up-to-date scientific literature on chemometrics, highlighting developments that have occurred since the first edition published Includes a new chapter devoted to new applications for state estimation in chemometrics Covers a new chapter entirely devoted to subspace identification methods Provides several new real-life examples of methods such as multiple modeling, principal component analysis, iterative target transformation factor analysis, and the generalized standard addition method

Food Authentication is an issue that has become increasingly important in recent years, due to the drive for more accurate and truthful labeling. This title provides a guide to the techniques available to establish food authenticity, together with their associated strengths and limitations. It is aimed at food scientists and technologists involved in the issues of adulteration or fortification of food and beverages.

Reviewing the analytical strategies used in the study of cultural heritage assets, this book pays particular attention to analytical methodology and ensuring reliable results are obtained for those working in conservation practice.

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