Book Review

Chemometrics: From Basics to Wavelet Transform. Chemical Analysis, Volume 164 By Foo-Tim Chau (Hong Kong Polytechnic University), Yi-Zeng Liang (Central South University), Junbin Gao (University of New England), and Xue-Guang Shao (University of Science and Technology of China). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. xiv + 316 pp. $99.95. ISBN 0-471-20242-8.

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J. Am. Chem. Soc., **2005**, 127 (7), 2365-2366• DOI: 10.1021/ja040937q • Publication Date (Web): 15 January 2005

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BOOK REVIEWS

Pseudo-Peptides in Drug Discovery. Edited by Peter E. Nielsen (University of Copenhagen). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany. 2004. xii + 244 pp. $125.00. ISBN 3-527-30633-1.

This book comprises six chapters contributed by leaders in the field of pseudo-peptides, although the emphasis is more academic than the words "Drug Discovery" in the title suggest. The first chapter, by Zuckermann et al., covers the peptoids (N-alkylated glycine oligomers) comprehensively, including syntheses, pharmaceutical applications, drug delivery, and issues of structure and conformation. Guichard takes on the ever-expanding area of β-peptides, γ-peptides, and isosteric backbones in the next chapter. This is necessarily long, but like Chapter 1, it appears to address all the important issues in this field. The chapter by Dervan and co-workers on pyrrole–imidazole polyamides is authoritative and beautifully illustrated with many color graphics. Nielsen et al. have a relatively short contribution on peptide nucleic acids (PNAs) that seems to emphasize the drug discovery aspect, whereas the chapter from Garner's group on α-helical PNAs stresses the biophysical features of these particular systems. There also is a chapter by Scarso and Scrimin that primarily deals with coordination complexes featuring peptides that cleave DNA or RNA.

Overall, the book is thoughtfully compiled and well-presented. Researchers working in these specific areas will want to own a copy of this book, and those of us interested in other types of peptidomimetics should encourage their libraries to get one.

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JA0409964

10.1021/ja0409964

Chemometrics: From Basics to Wavelet Transform. Chemical Analysis, Volume 164. By Foo-Tim Chau (Hong Kong Polytechnic University), Yi-Zeng Liang (Central South University), Junbin Gao (University of New England), and Xue-Guang Shao (University of Science and Technology of China). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. xiv + 316 pp. $99.95. ISBN 0-471-20242-8.

Chemometrics is an approach to analytical and measurement science that uses mathematical, statistical, and other methods of formal logic to determine (often by indirect means) the properties of substances that otherwise would be very difficult to measure directly. Much of the growth in this field is driven by demands that more information be extracted from data, the amount of which has increased dramatically because of the number and sophistication of chemical instruments. This increase has in turn triggered interest in the development of new techniques in data analysis that can extract information from the large arrays of chemical data routinely generated. As a result, the focus of chemometrics has shifted away from indirect observation and toward the science of analytical measurement. Placing chemical instrumentation under computer control has paved the way for development of new algorithms to optimize instrument performance. Resolving overlapping peaks, improving instrumental calibration, and classifying materials according to source are currently areas of active research in the field.

The authors of this volume attempt to explore the field of chemometrics through a recent development, the wavelet transform. Because wavelets can leverage information from data through denoising and compression, the wavelet transform plays an important role in the development of new algorithms to mine information from multivariate chemical data. This is reflected in the organization of the text, which is divided into five chapters. In the first chapter, the authors describe why chemometrics was developed and give a brief history of the field. They also enumerate, through worked examples, the challenges that analytical chemists must confront when analyzing their data and introduce the jargon of the field here, although they do not provide definitions for these terms. The authors conclude the chapter by presenting a brief introduction to wavelets and propose using them as a method for preprocessing chemical data, for example, removing a sloping baseline, enhancing signal-to-noise, data compression, etc. Commercial software for chemometrics is listed at the end of the chapter.

Chapter 2 focuses on signal processing techniques previously used for analytical data, which are represented as 1-D vectors, e.g., spectra and chromatograms. Moving average and Savitsky–Golay filtering techniques for enhancing signal-to-noise ratios are discussed, and MATLAB code for these two techniques and a worked example are provided. The relationship between Savitsky–Golay filtering and convolution techniques, such as Fourier and Hadamard transform techniques, is described, and the use of Fourier transform for denoising and data compression is elucidated. The chapter concludes with a discussion of principal component analysis for data compression. Although these techniques provide the reader with a suitable background for wavelets, other topics are interspersed throughout the chapter, e.g., Kalman filtering and cubic splines, which disrupt its logical flow.

In Chapter 3, the emphasis is on signal processing techniques used in multivariate curve resolution (MCR) for data obtained from so-called hyphenated methods. For this type of data, each sample is represented as a matrix of measurements. The properties of bilinear data are presented from the perspective of principal component analysis. Data preprocessing techniques for two-way data are treated, and methods for peak deconvolution are discussed, including evolving factor, window factor, and local rank analyses, as well as heuristic evolving latent projections. Unfortunately, the MCR methods that are described are no longer in vogue.

The wavelet transform and the wavelet packet transform, which are analogous to the Fourier transform, are the subject of Chapter 4. Because of their properties of localization, they are often preferred to Fourier transform in applications involving data compression, resolution, and signal enhancement of instrumental data. To explain wavelets, the authors first discuss the idea of decomposing a function or vector into templates or wavelets derived from a mother wavelet through scaling and translates. Then, the Haar wavelet is introduced, and its properties are enumerated in the context of spectral decomposition. After this, a summary of Mallat's algorithm for decomposition of multiresolution signals is presented, and a technique to construct wavelet functions is shown. Several examples of wavelet functions are presented, e.g., Meyer, B-spline, and Daubechies wavelets. The fast wavelet transform, which is used to express a signal in terms of the corresponding wavelet functions, and the inverse wavelet transform, which is used to reconstruct the signal from the remaining wavelet coefficients, are then explained. The chapter concludes with a discussion of the packet wavelet and the 2-D wavelet transform.

Chapter 5 focuses on applications of the wavelet transform to analytical chemistry. Examples are given illustrating data compression, denoising and smoothing, baseline/background removal, and resolution enhancement. Strategies are presented for the best way to implement each of these tasks. The worked examples focus on spectroscopic and chromatographic data. MATLAB codes for the examples presented can be obtained at the ftp server of the publisher, and a toolbox for developing wavelet programs can be found at Donoho's Stanford University Web site, whose URL is also provided. The chapter concludes with a survey of the analytical literature. In my opinion, this is the best chapter in the text because the authors are able to convey to the reader through worked examples the properties and unique attributes of wavelets. This chapter helps the reader to better understand the previous chapter, which is conceptual and abstract in nature.

The text is generally readable, but there are mistakes that detract from the presentation. For example, the authors state that hyphenated instrumentation is a recent advance even though GC−MS has existed for more than 30 years. Other deficiencies include referencing unpublished work to support important conclusions, the use of outdated concepts that neglect recent advances in the field, incorrect uses and interpretations of various types of data, and errors in explaining the mathematics of principal component analysis. In addition, the software on the publisher's Web site for the worked examples in the text could not be accessed. A more careful editing on the part of the publisher would have produced a more satisfying final product.

Despite these problems, my overall impression of the text is favorable. The authors have done a decent job of explaining wavelets. However, the material in the chapters preceding wavelets needs to be revised in any future edition in order to better reflect present trends in the field and to facilitate the logical flow of ideas crucial to understanding them. In conclusion, I would recommend this book to chemists who are interested in using wavelets in their research and to faculty who would like to teach graduate students about signal processing in a graduate course on optical spectroscopy.

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JA040937Q

10.1021/ja040937q