MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **83** (2020) 233-234

ISSN 0340 - 6253

BOOK REVIEW
Chemometrics – Statistics and Computer Application in Analytical Chemistry (3rd ed.)

by

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Wiley-VCH Verlag GmbH & Co. (2017), Print ISBN: 978-3-527-34097-2, ePDF ISBN: 978-3-527-69936-0

The book describes the chemometrics discipline developed from chemistry as a science. Chemometric methods are used for the "development of quantitative structure activity relationships and the evaluation of analytical–chemical data". Given the fact that the use of contemporary analytical instruments generates a large number of data, analytical chemists are motivated to use chemometric methods, i.e. mathematical and statistical methods underlying this discipline, by means of computer application. The main chapters of the book are as follows: (1) What is Chemometrics; (2) Basic Statistics; (3) Signal Processing and Time Series Analysis; (4) Optimization and Experimental Design; (5) Pattern Recognition and Classification; (6) Modeling; (7) Analytical Databases; (8) Knowledge Processing and Soft Computing; and (9) Quality Assurance and Good Laboratory Practice.

Chapter one is a presentation of the chemometrics discipline and is aimed at defining it and presenting "a way to count with bits and ways to perform arithmetic or logical operations in a computer".

The second chapter is entitled *Basic Statistics*, through a clarification of *Descriptive Statistics*, and within it the *Statistical Test and Analysis of*

Variance; this is followed by the third chapter, dealing with *Signal Processing and Time Series Analysis*, presenting this particular field through the two segments of the chapter, the one being Signal Processing and the other Time Series Analysis.

In the fourth chapter, the author points out the fact that "effective experimentation and the development of optimized methods are fundamental aims of any experimenter"; so, this chapter is dedicated to *Optimization and Experimental Design*.

The intention of Chapter 5 reflects in the introduction of the grouping of the analytical data based on unsupervised learning methods, and the handling of a multivariate along with the pattern recognition approaches, whereas Chapter 6 describes the models constructed and used in the analytics for the purpose of describing the relationship between responses and factors, and the calibration of analytical methods.

Chapter 7 is a presentation of Analytical Databases, first of all the Presentation of Analytical Information, so that, based on analytical data, an explanation could be given regarding the way how the spectrum and chemical structures in databases are coded and how searching in library-sources is conducted. Then, Chapter 8 clarifies the presentation and processing of knowledge in the computer so as to develop analytical expert systems, together with a presentation of genetical algorithms in order to solve complex problems. The intention of Chapter 9 is to present the metrics that will secure the quality of analytical-chemical measurement.

In brief: The book provides a practical and comprehensive account of the relatively new discipline of chemometrics through its two basic components: Statistics, and the use of Computer Application. It shows how chemometrics can efficiently be used in Analytical Chemistry. It can be a great source of information and a valuable guide for chemist research.

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