

BOOK REPORT

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Review of “Statistical Modelling of Molecular Descriptors in QSAR/QSPR” by Matthias Dehmer, Kurt Varmuza, and Danail Bonchev

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Book details

Statistical Modelling of Molecular Descriptors in QSAR/QSPR. Edited by Matthias Dehmer, Kurt Varmuza, and Danail Bonchev. Wiley-Blackwell, Weinheim, Germany, 2012. Print ISBN: 978-3-527-32434-7; ePDF ISBN: 978-3-527-64502-2. The book is Volume 2 of the series Quantitative and Network Biology. Series Editors: M. Dehmer and F. Emmert-Streib. Hard copy US\$ 159.95, Euros 129.99; E-book US\$ 126.00, Euros 114.00

The editors have selected 40 authors from 12 countries to contribute in producing a coherent account for the topics related to the book title. The 15 chapters of this book describe the current theoretical and practical results of statistical analysis and modelling of molecular descriptors. Zero-dimensional, 1-, 2-, and 3-dimensional descriptors are briefly mentioned. The most common 2D molecular descriptors are topological indices, and the use of any descriptor needs always a valid statistical confirmation that correlations are not due to chance. The first two chapters present, with some unavoidable overlap, introductory generalities about descriptors, various methods for modeling (multiple linear regression, partial least squares, neural networks, etc.) and for classification (linear discriminant analysis, k-nearest neighbor, support vector machine, etc.). Various software types are presented (e. g. Dragon, CODESSA, etc.).

The following chapters deal with more restricted aspects. In the 3rd chapter, after once again the software packages for descriptor calculation are reviewed, the Mold³ freeware is presented in detail, with a long list of all 777 descriptors. A few examples are described: in comparison with results obtained for classification (by Cerius², Dragon, and Molconn_Z) and regression models (by CODESSA), Mold² is seen to provide equal or better QSAR results. The 4th chapter is authored by V.

Consonni and R. Todeschini, who enumerate in detail all relevant graph-theoretical indices and who describe with loading plots how the classes of matrices and indices contained in the Dragon software reflect the principal components.

In chapter 5, A. G. Mercader and E. A. Castro describe the use of partial-order ranking and linear modeling for predictive QSAR/QSPR studies. They cite arguments showing that the enhanced or modified replacement methods yield superior results when compared to genetic algorithms. The authors describe how to select descriptors for ranking and constructing Hasse diagrams in order to illustrate partial ordering.

Descriptors for branched polymers and their uses for predicting gyration ratios and chain dynamics are described with mathematical rigor in Chapter 6. Chapter 7 presents methods for evaluating quantitatively structural similarity. Various clustering methods are also reviewed in this chapter by Irene Luque-Ruiz, G. Cerucla-García and M. A. Gómez-Nieto.

For compound database mining, Chapter 8 describes statistical methods for ligand-based virtual screening. In improving bioactive lead compound structures, the Kullback-Leibler divergence is used for quantifying the differences in value distributions of active and inactive compounds. Bayesian screening is exemplified in a recall prediction approach using the MACCS fingerprint.

In this reviewer's opinion, the 9th chapter on molecular descriptors and electronic structure is too long (48 pages). For instance, it presents on ten pages with half-page color plots trivial properties of the five hexane isomers, or it uses another half-page plot in order to prove lack of correlation, and fails to convey the more general and comprehensive aspects covered by the chapter's title.

By contrast, Chapter 10 by C. Kramer and T. Clark (12 pages) should have been longer because it presents new types of descriptors and models in SQAR/QSPR that are

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