PRIKAZ KNJIGE   **BOOK REVIEW**

James Devillers and Alexandru T. Balaban (Editors)
Topological Indices and Related Descriptors in QSAR and QSPR

This book, which is attractively designed and nicely printed, gives a state-of-art account of the theory of molecular descriptors and their uses in the quantitative structure-activity relationships (QSAR) and in the quantitative structure-property relationships (QSPR). The editors of this book, James Devillers (Centre de Traitement de l'Information Scientifique, Rillieux La Pape, France) and Alexandru T. Balaban (Department of Organic Chemistry, Faculty of Chemical Technology, Polytechnic University, Bucharest, Romania), are well-known contributors to the theory of molecular descriptors and their application in QSAR and QSPR. They succeeded in gathering a representative assembly of international authors for this book. The reader can learn how to compute descriptors from the structure of a molecule and the strategy of deriving QSAR and QSPR models.

The book consists of the Contents (pp. v–vi), Preface (pp. vii–viii), Contributors (pp. ix–x), 17 chapters (pp. 1–804) and Index (pp. 805–811).

The first chapter (pp. 1–20; 36 references), entitled »*No-Free Lunch Molecular Descriptors in QSAR and QSPR*«, was written by one of the editors, James Devillers. In this chapter, which is in a way an introductory chapter, the author stresses the advantages and limitations of different types of molecular descriptors that are presently in use in QSAR and QSPR in order to show that the universal molecular descriptor does not exist.

The second chapter (pp. 21–57; 151 references) is entitled »*Historical Development of Topological Indices*« and was written by the other editor, Alexandru T. Balaban, and Ovidiu Ivanciuc (Department of Organic Chemistry, Faculty of Chemical Technology, Polytechnic University, Bucharest, Romania). To my knowledge, this is the first, extensive account of the modern history of topological indices, which starts, according to the authors, with the

paper written by Harry Wiener when he was a chemistry student at the Brooklyn College (»Structural Determination of Paraffin Boiling Points«, *J. Am. Chem. Soc*. **69** (1947) 17–20).

The third chapter, which is the longest chapter (108 pages) in the book (pp. 59–167; 189 references), entitled »*The Graph Description of Chemical Structures*«, was written by the same authors as the preceding chapter, only the order of authors is reversed. In this chapter, the most important topological indices are reviewed, but the elements of graph theory, including the graph matrices, their spectra and polynomials, are also given.

The fourth chapter (pp. 169–220; 106 references) is entitled »*Vertex- and Edge-Weighted Molecular Graphs and Derived Structural Descriptors*« and was written by the Bucharest Group (O. Ivanciuc, T. Ivanciuc, A. T. Balaban). In this chapter, the authors describe how organic compounds containing heteroatoms, heterobonds and/or multiple bonds can be conveniently modeled by vertex- and edge-weighted molecular graphs. The main schemes proposed for computing the vertex- and edge-weighted graph parameters are reviewed and some examples are provided for the generation of the most important weighted graph matrices.

The fifth chapter (pp. 221–277; 120 references), entitled »*Matrices and Structural Descriptors Computed from Molecular Graph Distances*«, was again written by the members of the Bucharest Group (O. Ivanciuc, T. Ivanciuc). In this chapter, the authors describe a variety of (symmetric and nonsymmetric) distance matrices and the corresponding distance indices (for example, the Wiener index is the simplest distance index).

The sixth chapter (pp. 279–306; 54 references), which is entitled »*The Detour Matrix and the Detour Index*« and was written by Sonja Nikolić, Nenad Trinajstić (The Rugjer Bošković Institute, Zagreb, Croatia) and Zlatko Mihalić (Faculty of Science, University of Zagreb, Zagreb, Croatia), is closely related to the preceding chapter, because it deals with a special distance matrix, called the detour matrix, in which the longest graph distances enter as matrix elements. The detour index is derived from this matrix in the same way as the Wiener index is derived from the traditional distance matrix (in which the shortest graph distances enter as matrix elements), that is, it is equal to the sum of all elements in the upper- (lower-) half of the matrix.

The seventh chapter (pp. 307–360; 159 references), entitled »*Molecular Connectivity Chi Indices for Database Analysis and Structure-Property Modeling*«, was written by Lowell H. Hall (Department of Chemistry, Eastern Nazarene College, Quincy, MA, USA) and Lemont B. Kier (Department of Medicinal Chemistry, School of Pharmacy, Virginia Commonwealth University, Richmond, VA, USA), whose books (*Molecular Connectivity in Chemis-*

try and Drug Research, Academic Press, New York, 1976; Molecular Connectivity in Structure-Activity Analysis, Wiley, New York, 1986) contributed substantially to the early popularization of the use of topological indices in the structure-property-activity modeling. In this chapter, they employ the connectivity indices to invert QSAR equations in order to determine molecular structures that are predicted to possess activity values in a desired range.

The eighth chapter (pp. 361–401; 78 references) is entitled »*Overall Connectivity and Topological Complexity: A New Tool for QSPR/QSAR*« and was written by Danail Bonchev (Program for Theory of Complex Systems, Texas A&M University, Galveston, TX, USA and Assen Zlatarov University, Burgas, Bulgaria). In this chapter, the author, who is the foremost authority in the theory of complex systems, discusses the molecular complexity concepts, the related complexity indices and their uses in the structure-property modeling.

The ninth chapter (pp. 403–453; 159 references), entitled »*Novel Strategies in the Search of Topological Indices*«, was written by Ernesto Estrada (Department of Pharmacy, Universidad Central de Las Villas, Santa Clara, Villa Clara, Cuba). In this chapter, the author describes strategies for deriving topological indices based on edge properties and line graphs, on counting polynomials and topographic indices.

The next two chapters, tenth (pp. 455–489; 45 references) and eleventh (pp. 491–562; 42 references), entitled »*The Kappa Indices for Modeling Molecular Shape and Flexibility*« and »*The Electrotopological State: Structure Modeling for QSAR and Database Analysis*«, were both written by L. B. Kier and L. H. Hall. In the tenth chapter, they describe a series of non-empirical indices encoding information about molecular shape and flexibility, and in the eleventh chapter they present the electrotopological state as a method for encoding molecular structure at the atom level.

The twelfth chapter (pp. 563–593; 44 references), entitled »*Information Theoretic Indices of Neighborhood Complexity and Their Applications*«, was written by Subhash C. Basak (Natural Resources Research Institute, The University of Minnesota, Duluth, MN, USA). In this chapter, the author describes a set of complexity indices and their use in QSPR/QSAR studies.

The thirteenth chapter (pp. 595–612; 62 references), entitled »*Autocorrelation Descriptors for Modeling (Eco)Toxicological Endpoints*« and written by the first editor (J. Devillers), is the shortest chapter (18 pages) in the book. The author describes the autocorrelation method and its heuristic potency in toxicological modeling.

The fourteenth chapter (pp. 613–673; 77 references) is entitled »*DARC Site Topological Correlations: Ordered Structural Descriptors and Property*

Evaluation« and was written by the group of French authors: J.-E. Dubois, J. P. Doucet, A. Panaye and B. T. Fan (Institut de Topologie et de Dynamique des Systemes, Université Paris VII – Denis Diderot, Paris, France). The DARC (Description, Acquisition, Restitution, Computer-aided design) method and its uses are described.

The fifteenth chapter (pp. 675–696; 44 references) was written by the Duluth group (Subhash C. Basak, Brian D. Gute, Gregory D. Grunwald; Natural Resources Research Institute, The University of Minnesota, Duluth, MN, USA). The chapter is entitled »*A Hierarchical Approach to the Development of QSAR Models using Topological, Geometrical and Quantum Chemical Parameters*« and reports the development and uses of hierarchical QSPR/QSAR modeling.

The sixteenth chapter (pp. 697–777; 155 references), entitled »*Molecular Graph Descriptors Used in Neural Network Models*«, was written by Ovidiu Ivanciuc. This chapter describes the neural network modeling of molecular properties (physical, chemical, biological) using topological indices.

The seventeenth and last chapter in the book (pp. 779–804; 137 references) is entitled »*Algorithms and Software for the Computation of Topological Indices and Structure-Property Models*« and was written by Ovidu Ivanciuc and James Devillers. Several programs are reviewed, *e.g.*, GRAPH III (A. Sabljić, D. Horvatić, »GRAPH III: A Computer Program for Calculating Molecular Connectivity Indices on Microcomputers«, *J. Chem. Inf. Comput. Sci*. **33** (1993) 292–295), CODESSA (this program was developed by Alan R. Katritzky and his group at the University of Florida, Gainesville, FL, USA), TAM (M. Vedrina, S. Marković, M. Šarić-Medić, N. Trinajstić, »TAM: A Program for the Calculation of Topological Indices in QSPR and QSAR Studies«, *Comput. Chem.* **21** (1997) 355–361.), *etc*.

In the book, contributions are cited of a number of Croatian chemists, physicists, mathematicians, pharmaceutical and other scientists (Dragan Amić, Darko Babić, Dušanka Davidović-Amić, Željko Jeričević, Albin Jurić, Goran Krilov, Bono Lučić, Stribor Marković, Julija Matijević-Sosa, Marica Medić-Šarić, Zlatko Mihalić, Sonja Nikolić, Miroslava Protić, Milan Randić, Branko Ruščić, Dejan Plavšić, Aleksandar Sabljić, Slavko Šarić, Nenad Trinajstić, Mijo Vedrina, Darko Veljan, Tomislav Živković), since the development of topological indices and related descriptors and their uses in QSPR and QSAR modeling started in Croatia 30 years ago, at the time when only very few people elsewhere (Haruo Hosoya, Alexandru T. Balaban, Danail Bonchev, Jacques-Emile Dubois) were doing pioneering research in this field. Three times (p. 28, p. 678, p. 780) mention is made of two topological indices that were developed in Zagreb in 1973–1975, called the Zagreb group indices in honor of the theoretical chemistry group at the Rugjer Bošković Institute.

To conclude, we stress that this book will be a valuable reference for anyone involved in the use of QSPR and QSAR methodologies in chemistry, biochemistry, biology, toxicology, medicinal chemistry, drug design, engineering, pharmaceutical and environmental sciences and in teaching modeling techniques in a variety of undergraduate and graduate courses.

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Nenad Trinajstić
Sonja Nikolić

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