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BOOK REVIEW

R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Second, revised and enlarged edition. Wiley-VCH, Weinheim, 2009, ISBN 978-3-527-31852-0, Vol. 1: Alphabetical listing; Vol. 2: Appendices, references. $368.00. This monograph is part of the series *Methods and Principles of Medicinal Chemistry* (Vol. 41) edited by R. Mannhold, H. Kubinyi, and G. Folkers.

The second edition of the *Handbook of Molecular Descriptors*, which was published in 2000 by the same authors and publishing house, is a thoroughly revised and updated book: whereas the 2000 volume had 667 pages and included 3300 references, the present edition has two volumes with 967+252 pages, and the bibliography now includes about 6400 references involving almost 7000 authors and 450 periodicals.

In 1997 the authors had decided to write their *Handbook*, which took more than two years of full-time work; when it was published in 2000, two more monographs appeared in the same field, one authored by M. Karelson (Wiley), and another edited by J. Devillers and the present reviewer (Gordon and Breach). Of course, topological indices had been made widely known by the books published earlier by L. B. Kier and L. H. Hall. However, the book by Todeschini and Consonni has a different, encyclopedical organization, namely by alphabetical listing of topics, which are then described in detail. The present edition, with its changed title, keeps this organization but in addition to updating all information on new descriptors, QSAR/QSPR approaches and chemometric strategies for the years between the two editions, it also included many new entries such as biodescriptors for proteomes and genomes, property filters such as drug likeness, or scoring functions such as those used in substructure weights. Some topics have been completely rewritten in order to make this encyclopaedic guide to molecular descriptors usable for didactic purposes.

The idea of converting a chemical structural formula into a mathematical descriptor in order to help in quantitative correlations with biological activities (QSAR) or with other properties (QSPR) can be traced to A. Crum-Brown in the 1860s, one of the creators of structural formulas. Soon afterwards, W. Körner (Todeschini's great-grandfather) showed that the Kekulé formula allowed deducing the structure of disubstituted benzene derivatives by adding one more substituent:

formation of 1, 2, and 3 isomers indicates that the disubstitution was *para*, *ortho*, and *meta*, respectively. Then M. C. Richet, A. Y. Meyer and E. Overton at the end of the 19th century and first years of the 20th century found quantitative correlations between structure and biological or physical properties. However, the first topological indices (as term due to H. Hosoya) were introduced only in the 1940s by Wiener and Platt, allowing the conversion of a constitutional formula into a number that could be used in QSAR and QSPR (or the recently introduced related acronyms QMSA, QSAM, QSERR, QShAR, QSiAR, QSMR, QSRC, QSRR, QSTR, all explained at the end of Vol. 2).

In the Preface of Vol. 1, the authors mention that special attention was paid to strategies for generating families of molecular descriptors based on generalization of classical molecular descriptors such as Wiener-type, Randić-like, or Balaban-like indices. A citation from the Introduction presents the authors' view: *A molecular descriptor can be thought of as the mythological Dragon of the Babilon Ištar Gate (Pergamon Museum of Berlin), which actually is a mixing of several different animals, each corresponding to a different part of the Dragon body; likewise, a molecular descriptor has several different meanings which depend upon one's point of view.* It is relevant to mention that R. Todeschini's widely-used software is called *Dragon*; it is also worth mentioning that, in addition to the cited references, a thematic bibliography with almost 5000 entries is available as supplementary online material from the Wiley homepage.

Methods for processing molecular descriptors are based on statistics for validation of results, chemoinformatics and chemometrics. Drug resistance of germs makes it imperative to introduce often new and better medicinal drugs. The cost of a new drug on the market is awesome, and retiring a drug from the market may sometimes ruin a pharmaceutical company. No pharmaceutical research laboratory can withstand competition without theoretical tools for drug discovery, and molecular descriptors are the simplest, therefore least expensive, tools. Yet they are uncannily effective, as shown repeatedly by experience.

In conclusion, the present edition of the Todeschini-Consonni book is worthy having even when the previous edition is already available, because not only the title but also the contents are different in appreciable measure. In any case, future citations of this (already very well-cited) monumental work should refer from now on to the 2009 second revised and enlarged edition.

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