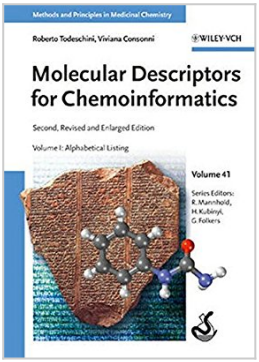

Molecular Descriptors for Chemoinformatics, Volume 41 (2 Volume Set) (Methods and Principles in Medicinal Chemistry)

By Roberto Todeschini, Viviana Consonni

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The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past six years has been painstakingly surveyed, resulting in hundreds of new descriptors being added to the list, and some 3,000 new references in the bibliography section. Volume 1 contains an alphabetical listing of more than 3300 descriptors and related terms for chemoinformatic analysis of chemical compound properties, while the second volume lists over 6,000 references selected from 450 journals. To make the data even more accessible, the introductory section has been completely re-written and now contains several "walk-through" reading lists of selected keywords for novice users.

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Editorial Review

Review
"Outstandingly succeeds in its aim, it really is a magnificent work and every scientific ad medical library and group linked to the field should have a copy." (Current Engineering Practice, 2011)

"The comprehensive listing of descriptors... is the actual strength of the book. Even experts in the field will find these sections helpful, because these are at the level of reviews." (*ChemMedChem*, 2010)"Outstandingly succeeds in its aim, it really is a magnificent work and every scientific ad medical library and group linked to the field should have a copy." (*Current Engineering Practice*, 2010)

“This is an outstanding book, a book that will be appreciated by many, not only today and in the near future, as is the case with most scientific books, but for years to come. I would like without any hesitation to strongly recommend this book as an essential ‘instrument’ in all chemometrics laboratories all over the world.” (*Journal of Chemical Information and Modeling*, January 2010)

From the Back Cover
As every chemist knows, there is a direct (if complex) relationship between the molecular structure of a compound and its chemical behavior. Predicting such behavior is possible by an abstract representation of its structure in terms of chemical similarity parameters, so-called 'descriptors'. These are most useful in predicting the pharmacological properties of drug candidates, but are also used in predicting reactivity, toxicity and other important chemical characteristics.
The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past six years has been painstakingly surveyed, resulting in more than 100 new descriptors being added to the list, and some 3,000 new references in the bibliography section.
Volume 1 contains an alphabetical listing of around 3300 terms for the chemoinformatic analysis of chemical compound properties, while the second volume contains 6343 references selected from 450 journals with about 7000 authors quoted covering the period from the beginning of molecular descriptor research until the year 2008.
In this second edition, the greatly expanded introductory section has been completely re-written and now contains several "walk-through" reading lists of selected keywords to make the data even more accessible for novice users.

About the Author
Roberto Todeschini is full professor of chemometrics at the Department of Environmental Sciences of the University of Milano-Bicocca (Milano, Italy), where he constituted the Milano Chemometrics and QSAR Research Group. His main research activities concern chemometrics in all its aspects, QSAR, molecular descriptors, multicriteria decision making and software development. President of the International Academy of Mathematical Chemistry, president of the Italian Chemometric Society and "ad honorem" professor of the University of Azuay (Cuenca, Ecuador), he is author of more than 170 publications in international journals and of the books "The Data Analysis Handbook", by I.E. Frank and R. Todeschini, 1994; and "Handbook of Molecular Descriptors", by R. Todeschini and V. Consonni, 2000.

Viviana Consonni received her PhD in chemical sciences from the University of Milano in 2000 and is now full researcher of chemometrics and chemoinformatics at the Department of Environmental Sciences of the

University of Milano-Bicocca (Milano, Italy). She is a member of the Milano Chemometrics and QSAR Research Group and has 10 years experience in multivariate analysis, QSAR, molecular descriptors, multicriteria decision making, and software development. She is author of more than 40 publications in peer-reviewed journals and of the book "Handbook of Molecular Descriptors," by R. Todeschini and V. Consonni, 2000. In 2006, she obtained the International Academy of Mathematical Chemistry Award for distinguished young researchers and, in June 2009, has been elected as youngest Member of the Academy.

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