DESCRIPTION

Quantitative studies on structure-activity and structure-property relationships are powerful tools in directed drug research. In recent years, various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors. It has become possible not only to assess diversities or similarities of structure databases, but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly increasing number of compound libraries. They even allow for a controlled de-novo design of new lead structures.

This is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day. This practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors. All descriptors are listed with their definition, symbols and labels, formulas, some numerical examples, data and molecular graphs, while numerous figures and tables aid comprehension of the definitions. Cross-references throughout, a list of acronyms and notations allow easy access to the information needed to solve a specific research problem. Examples of descriptor calculations along with tables of descriptor values for a set of selected reference compounds and an up-to-date reference list add to the practical value of the book, making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers.
ABOUT THE AUTHOR

Roberto Todeschini is full professor of chemometrics at the Department of Environmental Sciences of the University of Milano-Bicocca, 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 from 2008 to 2014, president of the Italian Chemometric Society and "ad honorem" professor of the University of Azuay, he is author of more than 170 publications on international journals and books. The latest is "Molecular Descriptors for Chemoinformatics" R. Todeschini and V. Consonni; Wiley-VCH, 2009.

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