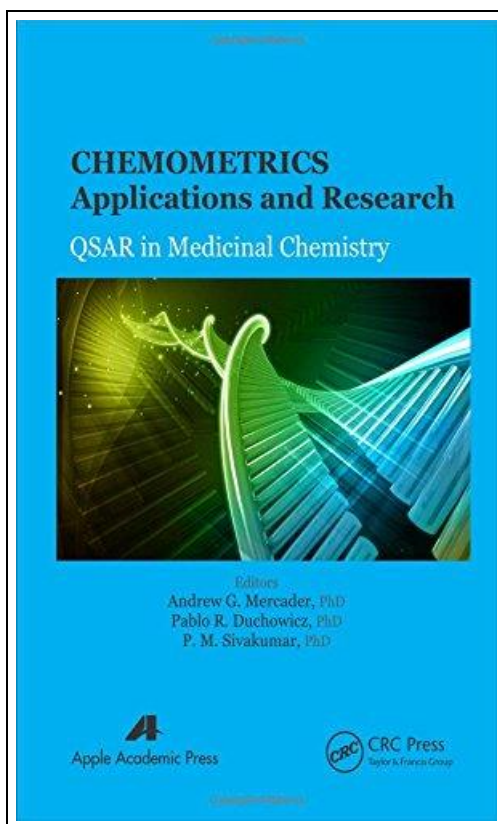


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Apple Academic Press Inc., Canada, 2016. Hardback. Condition: New. Language: English . Brand New Book. This important new book provides innovative material, including peer-reviewed chapters and survey articles on new applied research and development, in the scientifically important field of QSAR in medicinal chemistry. QSAR is a growing field because available computing power is continuously increasing, QSAR s potential is enormous, limited only by the quantity and quality of the available experimental input, which are also continuously improving. The number of possible structures for the design of new organic compounds is difficult to imagine, and QSAR helps to predict their activities even before synthesis. The book provides a wealth of valuable information and: * Presents an overview of recent developments in QSAR methodologies along with a brief history of QSAR * Covers the available web resource tools and in silico techniques used in virtual screening and drug discovery processes, compiling an extensive review of web resources in the following categories: databases related to chemical compounds, drug targets, and ADME/toxicity prediction; molecular modeling and drug designing; virtual screening; pharmacophore generation; molecular descriptor calculation software; software for quantum mechanics; ligand binding affinities (docking); and software related to ADME/toxicity prediction * Reviews the rm2 as a more stringent measure for the assessment of model predictivity compared to traditional validation metrics, being specifically important since validation is a crucial step in any QSAR study * Presents linear model improvement techniques that take into account the conformation flexibility of the modeled molecules * Summarizes the building processes of four different pharmacophore models: common-feature, 3D-QSAR, protein-, and protein-ligand complexes * Shows the role of different conceptual density functional theory based chemical reactivity descriptors, such as hardness, electrophilicity, net electrophilicity, and philicity in the design of different QSAR/QSPR/QSTR models * Reviews the use of chemometrics in PPAR...



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