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Nota di contenuto	Part I - Theoretical conceptions -- Fundamentals of mathematical modeling of chemicals through QSPR/QSAR -- Molecular descriptors in QSPR/QSAR modeling -- Application of SMILES to cheminformatics and generation of optimum SMILES descriptors using CORAL software -- Part II - SMILES based descriptors -- All SMILES Variational Autoencoder for Molecular Property Prediction and Optimization -- SMILES based bioactivity descriptors to model the anti-Dengue virus activity: A case study -- Part III - SMILES for QSPR/QSAR with optimal descriptors -- QSPR models for prediction of redox potentials using optimal descriptors -- Building up QSPR for polymers endpoints by using SMILES-based optimal descriptors -- Part IV - Quasi-SMILES for QSPR/QSAR -- Quasi-SMILES based QSPR/QSAR modeling -- Quasi-SMILES Based Mathematical Model for the Prediction of Percolation

Threshold for Conductive Polymer Composites -- On the possibility to build up the QSAR model of different kinds of inhibitory activity for a large list of Human Intestinal Transporter using quasi-SMILES -- Quasi-SMILES as a tool for peptide QSAR modelling -- Part V - SMILES and quasi-SMILES for QSPR/QSAR -- SMILES and quasi-SMILES descriptors in QSAR/QSPR modeling of diverse materials properties in safety and environment application -- SMILES and quasi-SMILES in QSAR Modeling for Prediction of Physicochemical and Biochemical Properties -- Part VI - Possible ways of nano-QSPR/nano-QSAR evolution -- The CORAL software as a tool to develop models for nanomaterials' endpoints -- Employing Quasi-SMILES notation in development of nano-QSPR models for nanofluids -- Part VII - Possible ways of QSPR/QSAR evolution in the future -- On complementary approaches of assessing the predictive potential of QSPR/QSAR-models -- CORAL: Predictions of Quality of Rice based on Retention index using a combination of Correlation intensity index and Consensus modelling.

Sommario/riassunto

This contributed volume overviews recently presented approaches for carrying out QSPR/QSAR analysis by using a simplifying molecular input-line entry system (SMILES) to represent the molecular structure. In contrast to traditional SMILES, quasi-SMILES is a sequence of special symbols-codes that reflect molecular features and codes of experimental conditions. SMILES and quasi-SMILES serve as a basis to develop QSPR/QSAR as well Nano-QSPR/QSAR via the Monte Carlo calculation that provides the so-called optimal descriptors for QSPR/QSAR models. The book presents a reliable technology for developing Nano-QSPR/QSAR while it also includes the description of the algorithms of the Monte Carlo optimization. It discusses the theory and practice of the technique of variational authodecoders (VAEs) based on SMILES and analyses in detail the index of ideality of correlation (IIC) and the correlation intensity index (CII) which are new criteria for the predictive potential of the model. The mathematical apparatus used is simple so that students of relevant specializations can easily follow. This volume is a valuable contribution to the field and will be of great interest to developers of models of physicochemical properties and biological activity, chemical technologists, and toxicologists involved in the area of drug design.