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| Nota di contenuto | Statistical Modelling of Molecular Descriptors in QSAR/QSPR; Contents; Preface; List of Contributors; 1 Current Modeling Methods Used in QSAR/QSPR; 1.1 Introduction; 1.2 Modeling Methods; 1.2.1 Methods for Regression Problems; 1.2.1.1 Multiple Linear Regression; 1.2.1.2 Partial Least Squares; 1.2.1.3 Feedforward Backpropagation Neural Network; 1.2.1.4 General Regression Neural Network; 1.2.1.5 Gaussian Processes; 1.2.2 Methods for Classification Problems; 1.2.2.1 Logistic Regression; 1.2.2.2 Linear Discriminant Analysis; 1.2.2.3 Decision Tree and Random Forest; 1.2.2.4 k-Nearest Neighbor<br>1.2.2.5 Probabilistic Neural Network1.2.2.6 Support Vector Machine; 1.3 Software for QSAR Development; 1.3.1 Structure Drawing or File Conversion; 1.3.2 3D Structure Generation; 1.3.3 Descriptor Calculation; 1.3.4 Modeling; 1.3.5 General purpose; 1.4 Conclusion; References; 2 Developing Best Practices for Descriptor-Based Property Prediction: Appropriate Matching of Datasets, Descriptors, Methods, |

and Expectations; 2.1 Introduction; 2.1.1 Posing the Question; 2.1.2 Validating the Models; 2.1.3 Interpreting the Models; 2.2 Leveraging Experimental Data and Understanding their Limitations
2.3 Descriptors: The Lexicon of QSARs2.3.1 Classical QSAR Descriptors and Uses; 2.3.2 Experimentally Derived Descriptors; 2.3.2.1 Biodescriptors; 2.3.2.2 Descriptors from Spectroscopy/Spectrometry and Microscopy; 2.3.3 0D, 1D and 2D Computational Descriptors; 2.3.4 3D Descriptors and Beyond; 2.3.5 Local Molecular Surface Property Descriptors; 2.3.6 Quantum Chemical Descriptors; 2.4 Machine Learning Methods: The Grammar of QSARs; 2.4.1 Principal Component Analysis; 2.4.2 Factor Analysis
2.4.3 Multidimensional Scaling, Stochastic Proximity Embedding, and Other Nonlinear Dimensionality Reduction Methods2.4.4 Clustering; 2.4.5 Partial Least Squares (PLS); 2.4.6 k-Nearest Neighbors (kNN); 2.4.7 Neural Networks; 2.4.8 Ensemble Models; 2.4.9 Decision Trees and Random Forests; 2.4.10 Kernel Methods; 2.4.11 Ranking Methods; 2.5 Defining Modeling Strategies: Putting It All Together; 2.6 Conclusions; References; 3 Mold2 Molecular Descriptors for QSAR; 3.1 Background; 3.1.1 History of QSAR; 3.1.2 Introduction to QSAR; 3.1.3 Molecular Descriptors: Bridge for QSAR
3.1.3.1 Molecular Descriptors3.1.3.2 Role of Molecular Descriptors; 3.1.3.3 Types of Molecular Descriptors; 3.1.3.4 Calculation of Molecular Descriptors (Software Packages); 3.2 Mold2 Molecular Descriptors; 3.2.1 Description of Mold2 Descriptors; 3.2.1.1 Topological Descriptors; 3.2.1.2 Constitutional Descriptors; 3.2.1.3 Information Content-based Descriptors; 3.2.2 Calculation of Mold2 Descriptors; 3.2.3 Evaluation of Mold2 Descriptors; 3.2.3.1 Information Content by Shannon Entropy Analysis; 3.2.3.2 Correlations between Descriptors; 3.3 QSAR Using Mold2 Descriptors
3.3.1 Classification Models based on Mold2 Descriptors

Sommario/riassunto

This handbook and ready reference presents a combination of statistical, information-theoretic, and data analysis methods to meet the challenge of designing empirical models involving molecular descriptors within bioinformatics. The topics range from investigating information processing in chemical and biological networks to studying statistical and information-theoretic techniques for analyzing chemical structures to employing data analysis and machine learning techniques for QSAR/QSPR.The high-profile international author and editor team ensures excellent coverage of the topic, making th