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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 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

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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