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Physicochemical Properties; 3.1 Introduction; 3.2 Prediction of Lipophilicity; 3.2.1 Fragment-Based Methods; 3.2.2 Methods Based on Molecular Properties; 3.2.3 Predictive Ability of Existing Techniques; 3.2.4 Other Solvent Systems; 3.2.5 Effect of Ionization
3.3 Prediction of Solubility 3.3.1 Fragmental Approaches; 3.3.2 Property-Based Methods; 3.3.3 Conclusions; 3.4 Prediction of pKa; 3.4.1 Fragment-Based Methods; 3.4.2 Methods Based on Molecular Properties; 3.4.3 Conclusions; 3.5 Prediction of Protein Binding; 3.6 Conclusions; References; 4 Descriptor-Based Similarity Measures for Screening Chemical Databases; 4.1 Introduction; 4.2 Fragment-Based Similarity Searching; 4.3 Association and Distance Coefficients for Similarity Searching; 4.4 Structural Representations for Similarity Searching; 4.4.1 Descriptor Selection; 4.4.2 Descriptor Encoding
4.5 Conclusions References; 5 Modelling Structure-Activity Relationships; 5.1 Introduction; 5.2 Hansch Analysis; 5.3 3-D QSAR; 5.4 Alignment-Free 3-D Descriptors; 5.5 Topological Descriptors; 5.6 Pharmacophores and Pharmacophoric Keys; 5.7 Conclusions; 5.8 Appendix - Statistical Techniques in QSAR and Pattern Recognition; 5.8.1 Data Reduction and Display; 5.8.1.1 Principal Component Analysis; 5.8.1.2 Non-Linear Mapping; 5.8.1.3 Neural Networks; 5.8.2 Regression Techniques; 5.8.2.1 Multiple Linear Regression; 5.8.2.2 Principal Component Regression and Partial Least Squares
5.8.3 Classification Techniques 5.8.3.1 Linear Discriminant Analysis; 5.8.3.2 Soft Independent Modelling of Class Analogy; 5.8.3.3 Recursive Partitioning; References; 6 Database Profiling by Neural Networks; 6.1 "Drug-Likeness": A General Compound Property?; 6.2 Methods and Programs; 6.2.1 Databases; 6.2.2 Descriptors; 6.2.3 Classification Tools; 6.2.4 Complete Algorithm; 6.3 Applications; 6.3.1 Drug-Likeness and a Recipe for a Computational Filter; 6.3.2 Crop Protection Compounds; 6.3.3 Virtual High-Throughput Screens; 6.3.4 Optimization of Combinatorial Libraries; 6.4 Conclusions; References
7 Pharmacophore Pattern Application in Virtual Screening. Library Design and QSAR

Sommario/riassunto

Recent progress in high-throughput screening, combinatorial chemistry and molecular biology has radically changed the approach to drug discovery in the pharmaceutical industry. New challenges in synthesis result in new analytical methods. At present, typically 100,000 to one million molecules have to be tested within a short period and, therefore, highly effective screening methods are necessary for today's researchers - preparing and characterizing one compound after another belongs to the past. Intelligent, computer-based search agents are needed and "virtual screening" provides solutions
