1. Record Nr. UNINA9910144110503321

Titolo	Virtual screening for bioactive molecules [[electronic resource] /] / edited by Hans-Joachim Bohm and Gisbert Schneider
Pubbl/distr/stampa	Weinheim ; ; New York, : Wiley-VCH, c2000
ISBN	1-282-01035-2 9786612010354 3-527-61308-0 3-527-61309-9
Descrizione fisica	1 online resource (327 p.)
Collana	Methods and principles in medicinal chemistry ; ; 10
Altri autori (Persone)	BohmHans-Joachim SchneiderGisbert <1965->
Disciplina	615 615.19 615.1900285 615/.19
Soggetti	Drugs - Design - Computer simulation Drugs - Testing - Computer simulation Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Virtual Screening for Bioactive Molecules; Preface; A Personal Foreword; Contents; List of Contributors; Prologue; 1 High-Throughput Screening and Virtual Screening: Entry Points to Drug Discovery; 1.1 Introduction; 1.2 Miniaturization and Detection Strategies; 1.2.1 Screening Plate Format and Fluidics; 1.2.2 Detection Strategies; 1.2.3 Cell-Based Reporter Gene Assays; 1.2.4 Fluorescence Correlation Spectroscopy .; 1.2.5 Microchip Fabrication; 1.2.6 Remarks and Summary; 1.3 Compound Libraries; 1.4 Multi-Dimensional Optimization: Qualifying HTS Lead Candidates; 1.5 Conclusions; References 2 Library Filtering Systems and Prediction of Drug-Like Properties2.1 Introduction; 2.2 Simple Counting Methods to Predict Drug-Likeness; 2.3 Functional Group Filters; 2.4 "Chemistry Space" Methods; 2.5 Examination of Building Blocks in Known Drugs; 2.6 Other Methods; 2.7 Conclusions and Future Directions; References; 3 Prediction of

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 Solubility3.3.1 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 ConclusionsReferences; 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 Techniques5.8.3.1 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

2. Record Nr. UNINA9910823851603321

Titolo	Biomedical data mining for information retrieval : methodologies, techniques, and applications / / edited by Sujata Dash [and three others]
Pubbl/distr/stampa	Hoboken, New Jersey ; ; Beverly, Massachusetts : , : Wiley : , : Scrivener Publishing, , [2021] ©2021
ISBN	1-119-71126-6 1-119-71127-4 1-119-71125-8
Descrizione fisica	1 online resource (448 pages)
Collana	Artificial intelligence and soft computing for industrial transformation
Disciplina	610.28
Soggetti	Biomedical engineering - Data processing
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.