

1. Record Nr.	UNISA996217063403316
Titolo	Advanced computer-assisted techniques in drug discovery [[electronic resource] /] / edited by Han van de Waterbeemd
Pubbl/distr/stampa	Weinheim ; ; New York, : VCH, c1995
ISBN	1-281-84288-5 9786611842888 3-527-61567-9 3-527-61566-0
Descrizione fisica	1 online resource (367 p.)
Collana	Methods and principles in medicinal chemistry ; ; v. 3
Altri autori (Persone)	WaterbeemdHan van de
Disciplina	615.10285 615.1900285
Soggetti	Pharmaceutical chemistry - Data processing Drugs - Design - Data processing Drugs - Research - Data processing QSAR (Biochemistry)
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	Advanced Computer- Assisted Techniques in Drug Discovery; Preface; A Personal Foreword; Contents; 1 Introduction; 1.1 3D QSAR; 1.2 Databases; 1.3 Progress in Multivariate Data Analysis; 1.4 Scope of this Book; References; 2 3D QSAR: The Integration of QSAR with Molecular Modeling; 2.1 Chemometrics and Molecular Modeling; 2.1.1 Introduction; 2.1.2 QSAR Methodology using Molecular Modeling and Chemometrics; 2.1.2.1 Search for the Geometric Pharmacophore; 2.1.2.2 Quantitative Correlation between Molecular Properties and Activity; 2.1.2.3 Computer Programs; 2.1.3 Illustrative Examples 2.1.3.1 Amnesia-Reversal Compounds2.1.3.2 Non-Peptide Angiotensin II Receptor Antagonists; 2.1.3.3 HMG-CoA Reductase Inhibitors; 2.1.3.4 Antagonists at the 5-HT3 Receptor; 2.1.3.5 Polychlorinated Dibenzo-p-dioxins; 2.1.4 Conclusions; References; 2.2 3D QSAR Methods; 2.2.1 Introduction; 2.2.2 3D QSAR of a Series of Calcium Channel Agonists; 2.2.2.1 Molecular Alignment; 2.2.2.2 Charges; 2.2.2.3 Generating 3D Fields; 2.2.2.4 Compilation of GRID Maps; 2.2.2.5 Inclusion of

Macroscopic Descriptors with 3D Field Data; 2.2.3 Statistical Analysis; 2.2.3.1 Results of the Analysis; 2.2.3.2 Testing the Model; 2.2.4 Conclusions; References; 2.3 GOLPE Philosophy and Applications in 3D QSAR; 2.3.1 Introduction; 2.3.1.1 3D Molecular Descriptors and Chemometric Tools; 2.3.1.2 Unfolding Three-way Matrices; 2.3.2 The GOLPE Philosophy; 2.3.2.1 Variable Selection; 2.3.3 Applications; 2.3.3.1 PCA on the Target Matrix; 2.3.3.2 PCA on the Probe Matrix; 2.3.3.3 PLS Analysis on the Target Matrix; 2.3.3.4 PLS on Target Matrix as a Strategy to Ascertain the Active Conformation; 2.3.3.5 GOLPE with Different 3D Descriptors; 2.3.4 Conclusions and Perspectives; References
 3 Rational Use of Chemical and Sequence Databases
 3.1 Molecular Similarity Analysis: Applications in Drug Discovery; 3.1.1 Introduction; 3.1.2 Similarity-Based Compound Selection; 3.1.2.1 Similarity Measures and Neighborhoods; 3.1.2.2 Application of 2D and 3D Similarity Measures; 3.1.2.3 Application of Dissimilarity-Based Compound Selection for Broad Screening; 3.1.3 Structure-Activity Maps (SAMs); 3.1.3.1 A Visual Analogy; 3.1.3.2 Representing Inter-Structure Distances; 3.1.3.3 Structure Maps; 3.1.3.4 Coloring a Structure Map; 3.1.4 Field-Based Similarity Methods
 3.1.4.1 Field-Based Similarity Measures; 3.1.4.2 Field-Based Molecular Superpositions; 3.1.4.3 An Example of Field-Based Fitting: Morphine and Clonidine; 3.1.5 Conclusions; References; 3.2 Clustering of Chemical Structure Databases for Compound Selection; 3.2.1 Introduction; 3.2.2 Review of Clustering Methods; 3.2.2.1 Hierarchical Clustering Methods; 3.2.2.2 Non-Hierarchical Clustering Methods; 3.2.3 Choice of Clustering Method; 3.2.3.1 Computational Requirements; 3.2.3.2 Cluster Shapes; 3.2.3.3 Comparative Studies; 3.2.4 Examples of the Selection of Compounds from Databases by Clustering Techniques

Sommario/riassunto

The use of powerful computers has revolutionized molecular design and drug discovery. Thoroughly researched and well-structured, this comprehensive handbook covers highly effective and efficient techniques in 3D-QSAR and advanced statistical analysis. The emphasis is on showing users how to apply these methods and avoid costly and time-consuming methodical errors. Topics covered include* combination of statistical methods and molecular modeling tools* rational use of databases* advanced statistical techniques* neural networks and expert systems in molecular design

2. Record Nr.	UNINA9910784255303321
Titolo	Advances and challenges in multisensor data and information processing [[electronic resource] /] / edited by Eric Lefebvre
Pubbl/distr/stampa	Amsterdam, Netherlands ; ; Washington, DC, : IOS Press, c2007
ISBN	6610934797 1-280-93479-4 9786610934799 1-60750-232-1 600-00-0327-7 1-4337-0858-2
Descrizione fisica	1 online resource (412 p.)
Collana	NATO security through science series. Sub-series D, Information and communication security, , 1574-5589 ; ; v. 8
Altri autori (Persone)	LefebvreEric <1968->
Disciplina	621.389/28
Soggetti	Multisensor data fusion Terrorism - Prevention Electronic surveillance
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"Published in cooperation with NATO Public Diplomacy Division." "Proceedings of the NATO Advanced Study Institute on Multisensor Data and Information Processing for Rapid and Robust Situation and Threat Assessment, Albena, Bulgaria, 16-27 May 2005"--T.p. verso.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Title page; Preface; Contents; Sensor Data Fusion: Methods, Applications, Examples; Simulation of Distributed Sensor Networks; Joint Target Tracking and Classification via Sequential Monte Carlo Filtering; A Survey on Assignment Techniques; Non-Linear Techniques in Target Tracking; Underwater Threat Source Localization: Processing Sensor Network TDOAs with a Terascale Optical Core Device; On Quality of Information in Multi-Source Fusion Environments; Polarimetric Features and Contextual Information Fusion for Automatic Target Detection and Recognition Enhancing Efficiency of Dynamic Threat Analysis for Combating and Competing Systems Evidence Theory for Robust Ship Identification in Airborne Maritime Surveillance Missions; Improved Threat Evaluation

Using Time of Earliest Weapon Release; Detection of Structural Changes in a Multivariate Data Using Change-Point Models; Unification of Fusion Theories (UFT); Belief Functions Theory for Multisensor Data Fusion; Dempster-Shafer Evidence Theory Through the Years: Limitations, Practical Examples, Variants Under Conflict and a New Adaptive Combination Rule
Decision Support and Information Fusion in the Context of Command and Control Fusion in European SMART Project on Space and Airborne Mined Area Reduction; The DSMT Approach for Information Fusion and Some Open Problems; Multitarget Tracking Applications of Dezert-Smarandache Theory; Image Registration: A Tutorial; Automated Registration for Fusion of Multiple Image Frames to Assist Improved Surveillance and Threat Assessment; Data Fusion and Image Processing: A Few Application Examples; Secondary Application Wireless Technologies to Increase Information Potential for Defence Against Terrorism
Adaptive Image Fusion Using Wavelets: Algorithms and System Design Methods for Fused Image Analysis and Assessment; Object Tracking by Particle Filtering Techniques in Video Sequences; Wavelets, Segmentation, Pixel- and Region- Based Image Fusion; Data Fusion and Quality Assessment of Fusion Products: Methods and Examples; Information Management Methods in Sensor Networks; A Novel Method for Correction of Distortions and Improvement of Information Content in Satellite-Acquired Multispectral Images; Multisensor Data Fusion in the Processes of Weighing and Classification of the Moving Vehicles Sensor Performance Estimation for Multi-Camera Ambient Security Systems: A Review Principles and Methods of Situation Assessment; Higher Level Fusion for Catastrophic Events; Ontology-Driven Knowledge Integration from Heterogeneous Sources for Operational Decision Making Support; Evaluation of Information Fusion Techniques Part 1 - System Level Assessment; Evaluation of Information Fusion Techniques Part 2 - Metrics; Rapid and Reliable Content Based Image Retrieval; Subject Index; Author Index

Sommario/riassunto

Information fusion resulting from multi-source processing is a relatively young technology domain. This book deals with the following research areas: Target recognition/classification and tracking; Sensor systems; Image processing; Remote sensing and remote control; Belief functions theory; and Situation assessment.
