1. Record Nr. UNINA9910830440503321

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 Model2.2.4 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
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3.1.4.1 Field-Based Similarity Measures3.1.4.2 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<br