1. Record Nr. UNINA9911020238503321

Titolo	Chemometric methods in molecular design / / edited by Han van de Waterbeemd
Pubbl/distr/stampa	Weinheim, Ger. ; ; New York, : VCH, c1995
ISBN	9786611758660 9781281758668 1281758663 9783527615452 3527615458 9783527615445 352761544X
Descrizione fisica	1 online resource (380 p.)
Collana	Methods and principles in medicinal chemistry ; ; v. 2
Altri autori (Persone)	WaterbeemdHan van de
Disciplina	547.13 615/.1901
Soggetti	QSAR (Biochemistry) Drugs - Design
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	Chernornetric Methods in Molecular Design; Preface; A Personal Foreword; Contents; 1 Introduction; 1.1 Quantitative Molecular Design; 1.2 Chemometrics; 1.3 The Hansch Approach; 1.4 Modern Chemometric Approaches in Molecular Design; 1.5 Software; 1.5.1 General Statistical Packages; 1.5.2 Specialized Software for SPC Studies; References; 2 Molecular Concepts; 2.1 Representations of Molecules; 2.1.1 Introduction; 2.1.2 Substituent Constants; 2.1.2.1 Electronic Substituent Constants; 2.1.2.2 The Hydrophobic Substituent Constant, p; 2.1.2.3 Partition Coefficient - Log P 2.1.2.4 Steric Substituent Constants2.1.3 Whole Molecule Representations; 2.1.3.1 Topological Descriptions; 2.1.3.2 Electronic Whole Molecule Descriptors; 2.1.3.3 Geometric Descriptors; References; 2.2 Atom-Level Descriptors for QSAR Analyzes; 2.2.1 Introduction; 2.2.2 An Atom-Level Description of Structure; 2.2.2.1 The Field; 2.2.2.2 The Intrinsic State of an Atom; 2.2.2.3 The Field Effect on Each Atom;

2.2.3 Strategies for Use of E-State Indices; 2.2.4 Examples of E-State QSAR; 2.2.4.1 MAO Inhibition with Hydrazides; 2.2.4.2 Adenosine A, Inhibitors
2.2.4.3 Anesthetic Concentration of Haloalkanes2.2.4.4 Odor Sensitivity of Pyrazines; 2.2.5 Conclusions; References; 3 Experimental Design in Synthesis Planning and Structure-Property Correlations; 3.1 Experimental Design; 3.1.1 The Importance of Experimental Design in Medicinal Chemistry; 3.1.2 Strategy in Experimental Design; 3.1.3 Selected Methods for Experimental Design; 3.1.3.1 Methods for the Direct Optimization of Lead Compounds; 3.1.3.2 Methods for the Systematic Investigation of Parameter Space; 3.1.3.3 Choice of Molecular Descriptors; 3.1.4 Summary and Conclusion; References
3.2 Applications of Statistical Experimental Design and PLS Modeling in QSAR3.2.1 Introduction; 3.2.2 A Strategy for QSAR Development in Drug Design; 3.2.2.1 Formulation of Classes of Similar Compounds (Step 1); 3.2.2.2 Structural Description and Definition of Design Variables (Step 2); 3.2.2.3 Selection of the Training Set of Compounds (Step 3); 3.2.2.4 Biological Testing (Step 4); 3.2.2.5 QSAR Development (Step 5; 3.2.2.6 Validation and Predictions for Non-Tested Compounds (Step; 3.2.3 Examples of Design and PLS Modeling; 3.2.3.1 Bradykinin Potentiating Pentapeptides
3.2.3.2 Dipeptides (Inhibiting the Angiotensin Converting Enzyme)
3.2.3.3 Dipeptides (Bitter Tasting); 3.2.3.4 Mimetics; 3.2.3.5 Haloalkanes; 3.2.3.6 Dibenzofurans; 3.2.3.7 Monosubstituted Benzenes; 3.2.3.8 Corrosive Carboxylic Acids; 3.2.4 Discussion and Conclusions; Software Used; Acknowledgements; References; 3.3 Total Response Surface Optimization; 3.3.1 Background; 3.3.2 Representation of a Response Surface; 3.3.3 Structure Descriptors from Chemical Graph Theory; 3.3.4 Examples; 3.3.4.1 Neurotoxicity of Fluorophosphorous Compounds
3.3.4.2 Bioconcentration of Chlorinated Phenyls and Biphenyls

Sommario/riassunto

The statistical analysis of experimental and theoretical data lies at the heart of modern drug design. This practice-oriented handbook is a comprehensive account of modern chemometric methods in molecular design. It presents strategies for making more rational choices in the planning of syntheses, and describes techniques for analyzing biological and chemical data. Written by the world's experts, it provides in-depth information on* molecular concepts* experimental design in the planning of syntheses* multivariate analysis of chemical and biological data* statistical validation