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Autore	Arguedas, José María
Titolo	Los ríos profundos / José María Arguedas ; edición de Ricardo González Vigil
Pubbl/distr/stampa	Madrid : Cátedra, 1995
ISBN	84-376-1321-3
Descrizione fisica	462 p. : ill. ; 18 cm
Collana	Letras Hispánicas ; 392
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Titolo	Protein-ligand interactions from molecular recognition to drug design / / edited by H.-J. Bohm and G. Schneider
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ISBN	1-280-52057-4 9786610520572 3-527-60551-7 3-527-60181-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (264 p.)
Collana	Methods and Principles in Medicinal Chemistry ; ; v.27
Altri autori (Persone)	BohmHans-Joachim SchneiderGisbert <1965->
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Note generali	Description based upon print version of record.
Nota di contenuto	Protein-Ligand Interactions From Molecular Recognition to Drug Design; Contents; Preface; A Personal Foreword; List of Contributors; List of Abbreviations; Prologue; 1 Prediction of Non-bonded Interactions in Drug Design; 1.1 Introduction; 1.2 Major Contributions to Protein-Ligand Interactions; 1.3 Description of Scoring Functions for Receptor-Ligand Interactions; 1.3.1 Force Field-based Methods; 1.3.2 Empirical Scoring Functions; 1.3.3 Knowledge-based Methods; 1.4 Some Limitations of Current Scoring Functions; 1.4.1 Influence of the Training Data; 1.4.2 Molecular Size 1.4.3 Water Structure and Protonation State1.5 Application of Scoring Functions in Virtual Screening and De Novo Design; 1.5.1 Successful Identification of Novel Leads Through Virtual Screening; 1.5.2 De novo Ligand Design with LUDI; 1.6 Outlook; 1.7 Acknowledgments; 1.8 References; 2 Introduction to Molecular Recognition Models; 2.1 Introduction and Scope; 2.2 Additivity of Pairwise Interactions - The Chelate Effect; 2.3 Geometric Fitting: The Hole-size Concept; 2.4 Di- and Polytopic Interactions: Change of Binding Mechanism with Different Fit; 2.5 Deviations from the Lock-and-Key Principle 2.5.1 Strain in Host-Guest Complexes2.5.2 Solvent Effects; 2.5.3 Enthalpy/Entropy Variations; 2.5.4 Loose Fit in Hydrophobically Driven Complex Formation; 2.6 Conformational Pre-organization: Flexible vs. Rigid Hosts; 2.7 Selectivity and Stability in Supramolecular Complexes; 2.8 Induced Fit, Cooperativity, and Allosteric Effects; 2.9 Quantification of Non-covalent Forces; 2.9.1 Ion Pairs and Electrostatic Donor-Acceptor Interactions; 2.9.2 Hydrogen Bonds; 2.9.3 Weak Hydrogen Bonds: The Use of Intramolecular ""Balances"; 2.9.4 Polarization Effects; 2.9.5 Dispersive Interactions 2.10 Conclusions2.11 References; 3 Experimental Approaches to Determine the Thermodynamics of Protein-Ligand Interactions; 3.1 Introduction; 3.2 Basic Thermodynamics of Protein-Ligand Interactions; 3.3 Measurement of Thermodynamic Parameters; 3.3.1 Calorimetric Determination of Thermodynamic Parameters; 3.3.2 van't Hoff Determination of Thermodynamic Parameters; 3.3.2.1 Relationship to Equilibrium Constant; 3.3.2.2 Obtaining the Equilibrium Constant; 3.4 Applications; 3.4.1 Calorimetric Determination of Thermodynamic Parameters; 3.4.2 van't Hoff Determination of Thermodynamic Parameters 3.5 Caveats3.6 Summary; 3.7 References; 4 The Biophore Concept; 4.1 Introduction; 4.2 Methodology for Pharmacophore Detection and Searching; 4.2.1 Definition of Pharmacophoric Groups; 4.2.2 Ligand-based Methods for Pharmacophore Perception; 4.2.3 Protein Structure-based Pharmacophore Perception; 4.2.4 Methods for Pharmacophore Searching; 4.3 Pharmacophore Fingerprints; 4.4 Applications of the Biophore Concept; 4.4.1 Lead Generation; 4.4.2 Multi-pharmacophore Descriptors in Diversity Analysis and Library Design; 4.4.3 Structure-based Design; 4.5 The Biophore Concept in ADME Prediction 4.6 Summary
Sommario/riassunto	The lock-and-key principle formulated by Emil Fischer as early as the end of the 19th century has still not lost any of its significance for the life sciences. The basic aspects of ligand-protein interaction may be summarized under the term 'molecular recognition' and concern the specificity as well as stability of ligand binding. Molecular recognition is thus a central topic in the development of active substances, since stability and specificity determine whether a substance can be used as a drug. Nowadays, computer-aided prediction and intelligent molecular

design make a large contributio