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Autore	Jantsch, Erich
Titolo	The self-organizing universe : scientific and human implications of the emerging paradigm of evolution / by Erich Jantsch
Pubbl/distr/stampa	Oxford [etc.], : Pergamon press, 1980
ISBN	0080243118 0080243126
Descrizione fisica	XVII, 343 p. : ill. ; 24 cm
Collana	Systems science and world order library. Innovations in systems science
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Autore	Holtje Hans-Dieter
Titolo	Molecular modeling : basic principles and applications / / Hans-Dieter Holtje and Gerd Folkers
Pubbl/distr/stampa	Weinheim, Germany ; ; New York, New York : , : John Wiley & Sons, , [1997] ©1997
ISBN	1-281-75846-9 9786611758462 3-527-61477-X 3-527-61476-1
Descrizione fisica	1 online resource (209 p.)
Collana	Methods and principles in medicinal chemistry ; ; v. 5
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Soggetti	Molecules - Models - Computer simulation Ligand binding (Biochemistry) - Computer simulation Biomolecules - Structure - Computer simulation Drugs - Design - Computer simulation
Lingua di pubblicazione	Inglese
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Molecular Modeling; Preface; A Personal Foreword; Contents; 1 Introduction; 1.1 Modern History of Molecular Modeling; 1.2 Do Today's Molecular Modeling Methods Illustrate only the Lukretian World?; 1.3 What are Models Used for?; 1.4 Molecular Modeling Uses All FourTypes for Model Building; 1.5 The Final Step is Design; 1.6 The Scope of the Book; 2 Small Molecules; 2.1 Generation of 3D Coordinates; 2.1.1 Crystal Data; 2.1.2 Fragment Libraries; 2.1.3 Sketch Approach; 2.2 Computational Tools for Geometry Optimization; 2.2.1 Force Fields; 2.2.2 Geometry Optimization 2.2.3 Energy-Minimizing Procedures2.2.3.1 Steepest Descent Minimizer; 2.2.3.2 Conjugate Gradient Method; 2.2.3.3 Newton-Raphson Minimizer; 2.2.4 Use of Charges, Solvation Effects; 2.2.5 Quantum Mechanical Methods; 2.2.5.1 Ab initio Methods; 2.2.5.2 Semiempirical Molecular Orbital Methods; 2.3 Conformational Analysis; 2.3.1 Conformational Analysis Using Systematic Search Procedures;

2.3.2 Conformational Analysis Using Monte Carlo Methods; 2.3.3 Conformational Analysis Using Molecular Dynamics; 2.4 Determination of Molecular Interaction Potentials
2.4.1 Molecular Electrostatic Potentials (MEPs)2.4.1.1 Methods for Calculating Atomic Point Charges; 2.4.1.2 Methods for Generating MEPs; 2.4.2 Molecular Interaction Fields; 2.4.2.1 Calculation of GRID Fields; 2.4.2.2 How GRID Fields can be Exploited; 2.4.2.3 Use of Chemometrics:The CoMFA Method; 2.4.3 Hydrophobic Interactions; 2.4.3.1 Log P as a Measure of Lipophilicity; 2.4.3.2 The Hydropathic Field; 2.4.3.3 Display of Properties on a Molecular Surface; 2.5 Pharmacophore Identification; 2.5.1 Molecules to be Matched; 2.5.2 Atom-by-Atom Superposition; 2.5.3 Superposition of Molecular Fields
2.6 The Use of Data Bants2.6.1 Conversion of 2D Structural Data into 3D Form; 2.6.2 3D Searching; 3 Example for Small Molecule Modeling: Serotonin Receptor Ligands; 3.1 Definition of the Serotoninergic Pharmacophore; 3.2 The Molecular Interaction Field; 3.3 Construction of a 5-HT 2a Receptor Binding Site Model; 3.4 Calculation of Interaction Energies; 3.5 Validation of the Model; 4 Introduction to Protein Modeling; 4.1 Where and How to get Information on Proteins; 4.2 Terminology and Principles of Protein Structure; 4.2.1 Conformational Properties of Proteins
4.2.2 Types of Secondary Structural Elements4.2.2.1 The -Helix; 4.2.2.2 The -Sheet; 4.2.2.3 Turns; 4.2.3 Homologous Proteins; 4.3 Knowledge-Based Protein Modeling; 4.3.1 Procedures for Sequence Alignments; 4.3.2 Determination and Generation of Structurally Conserved Regions (SCRs); 4.3.3 Construction of Structurally Variable Regions (SVRs); 4.3.4 Side Chain Modeling; 4.3.5 Distance Geometry Approach; 4.3.6 Secondary Structure Prediction; 4.3.7 Energy-Based Modeling Methods; 4.4 Optimization Procedures - Model Refinement - Molecular Dynamics; 4.4.1 Force Fields for Protein Modeling
4.4.2 Geometry Optimization

Sommario/riassunto

Written by experienced experts in molecular modeling, this books describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations. Its main objective is the description of the various pitfalls to be avoided. Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules.A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work!