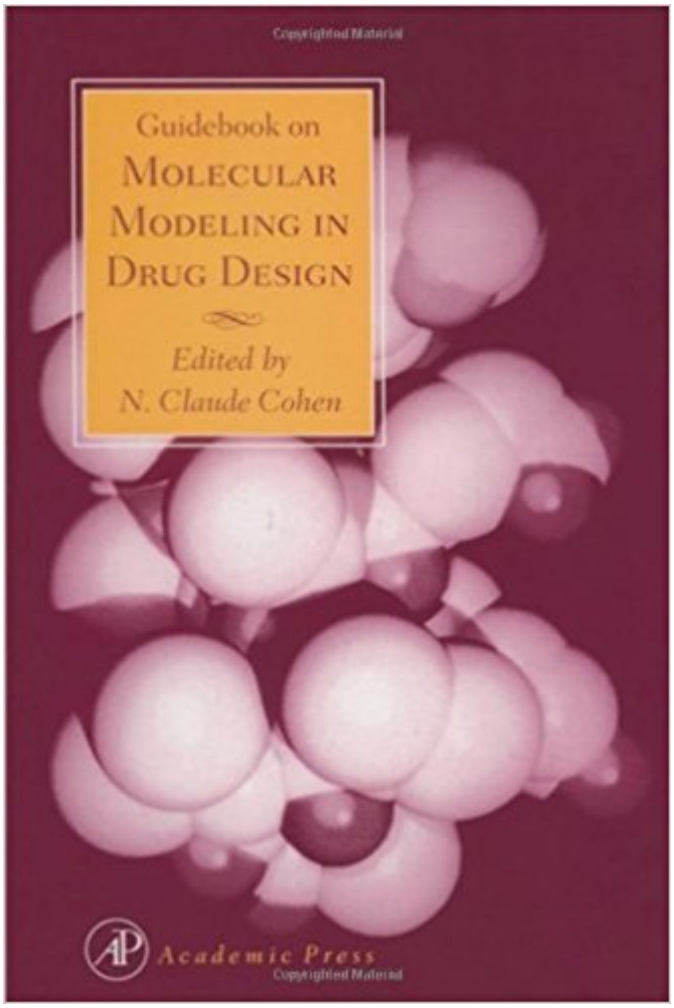
Guidebook On Molecular Modeling In Drug Design



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Specially designed computer software is revolutionizing procedures for structured or rational drug design and discovery. The Guidebook on Molecular Modeling in Drug Design serves as a manual for the analysis ofmolecular structure and the correlation of these structures with pharmacological reactions. Intended as an introductory guide for advanced students and professionals with an interest in computer-assisted modeling for drug design and discovery, this bookwill also be of interest to medicinal and organic chemists, pharmaceutical researchers, pharmacologists, and biochemists who want to gain further insight into this rapidly advancing field.Molecular modeling is assuming an important role in the understanding of three-dimensional aspects in the specificity of drug-receptor interactions at the molecular level. This research area has become a well-established discipline in pharmaceutical research. It has created unprecedented opportunities in assisting medicinal chemists in the design of new therapeutic agents. Advances made in computer hardware and in theoretical medicinal chemistry have brought high-performance computing and graphics tools within reach of most academic and industrial laboratories, facilitating the development of useful approaches to rational drug design.The Guidebook on Molecular Modeling in Drug Design serves as a manual for the analysis of the molecular structure of biological molecules and drugs and the correlation of these structures with pharmacological actions. Intended as a guide for advanced

students and professionals with an interest in computer-assisted modeling for drug design and discovery, this book will also be of interest to medicinal and organic chemists, pharmaceutical researchers, pharmacologists, and biochemists who want to gain further insight into this rapidly advancing field.

This book is structured as set of monographs by different authors, apparently invited specifically for this book. That's a format with strengths but also some serious weaknesses.First, the strengths. The seven chapters, plus a glossary chapter, cover a fair bit of ground. The chapter on computation hardware and graphics started aging the day it was written, but the other chapters all offer insights. The topics are varied, and include basics of docking, a nice intro to crystallization and crystallography, a description of the approval process and the team required, and a description of several trails from target molecule and native ligand to serious drug candidate. The glossary is worthwhile, and could have been expanded well beyond its 19 pages.The weakness of this format is that, although each chapter contains introductory material, the book as a whole is not written at the introductory level. It's not quite a text, more like seven unrelated chapters flying in close formation. No one, clear underlying pattern unifies the different piece. Maybe there is a pattern, but the reader must know it already. But in that case, would the reader really need the introductions? Also, the glossary was written without respect to the other chapters so isn't really a glossary of the book that contains it.Finally, I have to point out that this book's copyright date of 1996 makes it a bit old, by the standards of the field.There are a number of interesting facts to be had here. They are all isolated points, though. The reader must already have a pretty good idea of the whole picture that these points fit into.

The book emphasis is on different drug design techniques, specifically; The molecular modeling perspective in drug design, Molecular graphics and modeling, Molecular modeling of small molecules, Computer-assisted new lead design, Experimental techniques and data banks, Computer-assisted drug discovery, and Modeling drug-receptor interactions. The book covers in depth the docking of small molecules with protein receptors. Also the book surveys the molecular modeling packages currently used, their usage, strengths and weaknesses. The two main weaknesses of this book are (1) few illustrative figrues, (2) subjects overlapping (due to the fact that a group of authors contributed in writing this book). The book is really a guide book on molecular modeling and drug design as the title suggested.

Guidebook on Molecular Modeling in Drug Design Molecular Simulation Studies on Thermophysical Properties: With Application to Working Fluids (Molecular Modeling and Simulation) Molecular Visions Organic Model Kit with Molecular Modeling Handbook Drug Addicts- Prescription Pill Drug Abuse: How to Deal With an Addict Adult, Friend, Family Member, Teen or Teenager Who is Addicted to Medications (Prescription Pill Drug Abuse Help) Crystallographic and Modeling Methods in Molecular Design Graphic Design Success: Over 100 Tips for Beginners in Graphic Design: Graphic Design Basics for Beginners, Save Time and Jump Start Your Success (graphic ... graphic design beginner, design skills) Essentials of Molecular Pharmacology: Background for Drug Design Molecular Similarity in Drug Design Molecular Quantum Similarity in QSAR and Drug Design (Lecture Notes in Chemistry) The Organic Chemistry of Drug Design and Drug Action The Organic Chemistry of Drug Design and Drug Action, Second Edition The Organic Chemistry of Drug Design and Drug Action, Third Edition The Model's Bible & Global Modeling Agency Contact List - An Insider's Guide on How to Break into the Fashion Modeling Industry Modeling Agency Tips: Get Listed with Fashion Modeling Agencies and Find Your Dream Job 3ds Max Modeling for Games: Insider's Guide to Game Character, Vehicle, and Environment Modeling: Volume I Atmospheric and Space Flight Dynamics: Modeling and Simulation with MATLABÂ® and SimulinkÂ® (Modeling and Simulation in Science, Engineering and Technology) Introduction to the Numerical Modeling of Groundwater and Geothermal Systems: Fundamentals of Mass, Energy and Solute Transport in Poroelastic Rocks (Multiphysics Modeling) Modeling Dynamic Biological Systems (Modeling Dynamic Systems) Dynamic Modeling in the Health Sciences (Modeling Dynamic Systems) 3ds Max Modeling for Games: Insider's Guide to Game Character, Vehicle, and Environment Modeling: 1