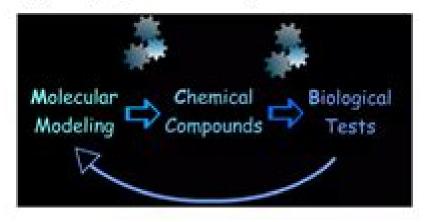
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David B. Weiner, William V. Williams

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Weaver, 2005-08-11 Fully updated and rewritten by a basic scientist who is also a practicing physician the third edition of this popular textbook remains comprehensive authoritative and readable Taking a receptor based target centered approach it presents the concepts central to the study of drug action in a logical mechanistic way grounded on molecular and principles Students of pharmacy chemistry and pharmacology as well as researchers interested in a better understanding of drug design will find this book an invaluable resource Starting with an overview of basic principles Medicinal Chemistry examines the properties of drug molecules the characteristics of drug receptors and the nature of drug receptor interactions Then it systematically examines the various families of receptors involved in human disease and drug design The first three classes of receptors are related to endogenous molecules neurotransmitters hormones and immunomodulators Next receptors associated with cellular organelles mitochondria cell nucleus endogenous macromolecules membrane proteins cytoplasmic enzymes and pathogens viruses bacteria are examined Through this evaluation of receptors all the main types of human disease and all major categories of drugs are considered. There have been many changes in the third edition including a new chapter on the immune system Because of their increasingly prominent role in drug discovery molecular modeling techniques high throughput screening neuropharmacology and genetics genomics are given much more attention. The chapter on hormonal therapies has been thoroughly updated and re organized Emerging enzyme targets in drug design e g kinases caspases are discussed and recent information on voltage gated and ligand gated ion channels has been incorporated The sections on antihypertensive antiviral antibacterial anti inflammatory antiarrhythmic and anticancer drugs as well as treatments for hyperlipidemia and peptic ulcer have been substantially expanded One new feature will enhance the book s appeal to all readers clinical molecular interface sections that facilitate understanding of the treatment of human disease at a molecular level Chemical and Structural Approaches to Rational Drug Design David B. Weiner, William V. Williams, 2020-12-18 This book is the first to provide both a broad overview of the current methodologies being applied to drug design and in depth analyses of progress in specific fields It details state of the art approaches to pharmaceutical development currently used by some of the world's foremost laboratories. The book features contributors from a variety of fields new techniques previously unpublished data and extensive reference lists Theoretical Aspects of Rational Drug Design (RDD): An Overview Supratim Ray, 2012-09-22 Medicinal Chemistry Thomas Nogrady, Donald F. Weaver, 2005-08-11 Fully updated this textbook takes a receptor based target centred approach presenting concepts central to the study of drug action in a logical mechanistic way grounded on molecular biochemical principles Guidebook on Molecular Modeling in Drug Design N. Claude Cohen, 1996-04-26 The molecular modeling perspective in drug design N Calude Cohen Molecular graphics and modeling tools of the trade Roderick E Hubbard Molecular modeling of small molecules Tamara Gund Computer assisted new lead design Akiko Itai Miho Yamada Mizutani Yoshihiko Nishibata and Nubuo Tomioka Experimental techniques and data banks John P Priestle and C Gregory Paris Computer assisted drug

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Chemical Drug Design Girish Kumar Gupta, Vinod Kumar, 2016-10-10 Chemical Drug Design provides a compact overview on recent advances in this rapidly developing field With contributions on in silico drug design natural product based compounds as well as on ligand and structure based approaches the authors present innovative methods and techniques for identifying and synthetically designing novel drugs Rational Drug Design Donald G Truhlar, W. Jeffrey Howe, Anthony J Innovations and Implementations of Computer Aided Drug Discovery Strategies in Rational Drug Hopfinger, 1999-03-12 Design Sanjeev Kumar Singh, 2021-02-02 This book presents various computer aided drug discovery methods for the design and development of ligand and structure based drug molecules A wide variety of computational approaches are now being used in various stages of drug discovery and development as well as in clinical studies Yet despite the rapid advances in computer software and hardware combined with the exponential growth in the available biological information there are many challenges that still need to be addressed as this book shows In turn it shares valuable insights into receptor ligand interactions in connection with various biological functions and human diseases The book discusses a wide range of phylogenetic methods and highlights the applications of Molecular Dynamics Simulation in the drug discovery process It also explores the application of quantum mechanics in order to provide better accuracy when calculating protein ligand binding interactions and predicting binding affinities In closing the book provides illustrative descriptions of major challenges associated with computer aided drug discovery for the development of therapeutic drugs Given its scope it offers a valuable asset for life sciences researchers medicinal chemists and bioinformaticians looking for the latest information on computer aided methodologies for drug development together with their applications in drug discovery

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