

Rational Drug Design -

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Rational Drug Design

David B. Weiner, William V. Williams



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This primary textbook for a first course in pharmacology offers an integrated systems based and mechanism based approach to understanding drug therapy Each chapter focuses on a target organ system begins with a clinical case and incorporates cell biology biochemistry physiology and pathophysiology to explain how and why different drug classes are effective for diseases in that organ system Over 400 two color illustrations show molecular cellular biochemical and pathophysiologic processes underlying diseases and depict targets of drug therapy Each Second Edition chapter includes a drug summary table presenting mechanism clinical applications adverse effects contraindications and therapeutic considerations New chapters explain how drugs produce adverse effects and describe the life cycle of drug development The fully searchable online text and an image bank are available on thePoint *Medicinal Chemistry* Thomas Nogrady, Donald F.

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

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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

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for all the institutions communities and individuals involved in the conservation use study and commercialisation of genetic resources *Protein Crystallography in Drug Discovery, Volume 20* Robert E. Babine, Sherin S. Abdel-Meguid, 2004-02-13

The rational structure based approach has become standard in present day drug design As a consequence the availability of high resolution structures of target proteins is more often than not the basis for an entire drug development program Protein structures suited for rational drug design are almost exclusively derived from crystallographic studies and drug developers are relying heavily on the power of this method Here researchers from leading pharmaceutical companies present valuable first hand information much of it published for the first time They discuss strategies to derive high resolution structures for such important target protein classes as kinases or proteases as well as selected examples of successful protein crystallographic studies A special section on recent methodological developments such as for high throughput crystallography and microcrystallization is also included A valuable companion for crystallographers involved in protein structure determination as well as drug developers pursuing the structure based approach for use in their daily work

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 Hopfinger, 1999-03-12 *Innovations and Implementations of Computer Aided Drug Discovery Strategies in Rational Drug 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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