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Computer **Applications** in Pharmaceutical Research and Development

Sean Ekins

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Carbon Monoxide in Drug Discovery Binghe Wang, Leo E. Otterbein, 2022-06-01 CARBON MONOXIDE IN DRUG DISCOVERY An insightful reference for the latest physiological and therapeutic studies of carbon monoxide In Carbon Monoxide in Drug Discovery Basics Pharmacology and Therapeutic Potential a team of distinguished authors delivers foundational knowledge the latest research and remaining challenges regarding the physiological roles and therapeutic efficacy of carbon monoxide CO The editors have included a broad selection of resources from leading experts in the field that discuss the background and physiological roles of CO a variety of delivery forms including CO prodrugs using benign carriers CO sensing therapeutic applications and clinical trials Organized by topic to allow each chapter to be read individually the book covers a wide range of topics from physiological and patho physiological mechanisms at the molecular level to clinical applications for multiple disease processes The editors of Carbon Monoxide in Drug Discovery have created a compelling argument for shifting the accepted understanding of CO from poison to bioactive molecule with enormous clinical benefits Readers will also benefit from A thorough introduction to the background and physiological actions of carbon monoxide including endogenous CO production in sickness and in health Comprehensive explorations of CO delivery forms including non carrier formulations metal carbonyl complexes and organic CO donors Practical discussions of carbon monoxide sensing and scavenging including fluorescent probes for intracellular carbon monoxide detection In depth examinations of the therapeutic applications of CO including CO in solid organ transplantation Perfect for professors graduate students and postdocs in the fields of biology pharmacology immunology medicinal chemistry toxicology and drug delivery Carbon Monoxide in Drug Discovery Basics Pharmacology and Therapeutic Potential is also an invaluable resource for industrial scientists in these areas Computer Applications in Drug Discovery and Development Ayarivan Puratchikody, Sakthivel Lakshmana Prabu, Appavoo Umamaheswari, 2018-11-23 With more restrictions upon animal experimentations pharmaceutical industries are currently focusing on a new generation of experiments and technologies that are considerably more efficient and less controversial The integration of computational and experimental strategies has led to the identification and development of promising compounds Computer Applications in Drug Discovery and Development is a pivotal reference source that provides innovative research on the application of computers for discovering and designing new drugs in modern molecular biology and medicinal chemistry While highlighting topics such as chemical structure databases and dataset utilization this publication delves into the current panorama of drug discovery where high drug failure rates are a major concern and properly designed virtual screening strategies can be a time saving cost effective and productive alternative This book is ideally designed for chemical engineers pharmacists molecular biologists students

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explains the principles structure and format of LCC details notation tables assigning class numbers and individual classes

and covers classification of special types of library materials The last chapter of this perennially useful resource addresses the potential role of classification in libraries of the future HIV-1 Integrase Nouri Neamati, 2011-08-10 This book comprehensively covers the mechanisms of action and inhibitor design for HIV 1 integrase It serves as a resource for scientists facing challenging drug design issues and researchers in antiviral drug discovery Despite numerous review articles and isolated book chapters dealing with HIV 1 integrase there has not been a single source for those working to devise anti AIDS drugs against this promising target But this book fills that gap and offers a valuable introduction to the field for the interdisciplinary scientists who will need to work together to design drugs that target HIV 1 integrase Strategies David J. Livingstone, Andrew M. Davis, 2012 This book shows how various facets of the drug discovery process can be addressed in a quantitative fashion Biophysical and Computational Tools in Drug Discovery Anil Kumar Saxena, 2021-10-18 This book reviews recent physicochemical and biophysical techniques applied in drug discovery research and it outlines the latest advances in computational drug design Divided into 10 chapters the book discusses about the role of structural biology in drug discovery and offers useful application cases of several biophysical and computational methods including time resolved fluorometry TRF with F rster resonance energy transfer FRET X Ray crystallography nuclear magnetic resonance spectroscopy mass spectroscopy generative machine learning for inverse molecular design quantum mechanics molecular mechanics QM MM ONIOM and quantum molecular dynamics QMT methods Particular attention is given to computational search techniques applied to peptide vaccines using novel mathematical descriptors and structure and ligand based virtual screening techniques in drug discovery research Given its scope the book is a valuable resource for students researchers and professionals from pharmaceutical industry interested in drug design and discovery **Transporters** Guofeng You, Marilyn E. Morris, 2014-07-07 This new edition overviews drug transporters and presents the principles of drug transport and associated techniques featuring new chapters on multidrug and toxin extrusion proteins placental transport in silico approaches in drug discovery and regulatory guidance for drug transport studies in drug development Describes drug transporter families mechanisms and clinical implications along with experimental methods for studying and characterizing drug transporters Includes new chapters on multidrug and toxin extrusion proteins placental transport and in silico approaches in drug discovery Has a new chapter covering regulatory guidance for the evaluation of drug transport in drug development with global criteria used for drug transporters in clinical trials Arranges material to go from fundamental mechanisms to clinical outcomes making the book useful for novice and expert readers **Translational** Bioinformatics and Its Application Dong-Qing Wei, Yilong Ma, William C.S. Cho, Qin Xu, Fengfeng Zhou, 2017-03-31 This book offers a detailed overview of translational bioinformatics together with real case applications Translational bioinformatics integrates the areas of basic bioinformatics clinical informatics statistical genetics and informatics in order to further our understanding of the molecular basis of diseases By analyzing voluminous amounts of molecular and clinical data

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Polysaccharide based Nano-Biocarrier in Drug Delivery Tapan Kumar Giri, Bijaya Ghosh, 2018-09-03 This book discusses various fundamental aspects of polysaccharide based nano biocarrier drug delivery systems and its application in the delivery of small molecules proteins peptides oligonucleotides and genes It also discusses advances in drug delivery systems in treatment of cancer cardiovascular pulmonary and infectious diseases

Cyclic-Nucleotide Phosphodiesterases in the Central Nervous System Nicholas J. Brandon, Anthony R. West, 2014-03-07 This book reviews advances in understanding phosphodiesterases within the central nervous system and their therapeutic applications A range of expert authors from both academia and industry describe these then focus on the areas of greatest scientific and medical interest to provide more detailed coverage Therapeutic and drug discovery applications are covered for diseases including Alzheimer's Parkinson's schizophrenia erectile dysfunction and spinal cord injuries There is also a chapter on drug discovery tools such as in vitro assays and X ray structures for medicinal chemistry studies

Dendrimer-Based Drug Delivery Systems Yiyun Cheng, 2012-07-03 The opportunities and challenges of using dendrimers to improve drug delivery Among pharmaceutical and biomedical researchers the use of dendrimers in drug delivery systems has attracted increasing interest In particular researchers have noted that the volume of a dendrimer increases when it has a positive charge If this property can be applied effectively dendrimers have enormous potential in drug delivery systems directly supplying medication to targeted human organs With contributions from an international team of pioneers and experts in dendrimer research this book provides a comprehensive overview of the latest research efforts in designing and optimizing dendrimer based drug delivery systems. The book analyzes key issues demonstrating the critical connections that link fundamental concepts design synthesis analytical methodology and biological assessment to the practical use of dendrimers in drug delivery applications Topics covered include Dendrimer history Synthesis Physicochemical properties Principles of drug delivery Applications in diverse biomedical fields Dendrimer Based Drug Delivery Systems reflects the authors thorough review and analysis of the current literature as well as their own firsthand experience in the lab Readers will not only discover the current state of the science but also gain valuable insights into fruitful directions for future research References at the end of each chapter serve as a gateway to the growing body of literature in the field enabling readers to explore each individual topic in greater depth Pharmaceutical and biomedical researchers will find this book a unique and essential guide to the opportunities issues and challenges involved in fully exploiting the potential of dendrimers to improve drug delivery **Applied Chemoinformatics** Thomas Engel, Johann Gasteiger, 2018-06-05 Edited by world famous pioneers in chemoinformatics this is a clearly structured and applications oriented approach to the topic providing up to date and focused information on the wide range of applications in this exciting

field The authors explain methods and software tools such that the reader will not only learn the basics but also how to use the different software packages available Experts describe applications in such different fields as structure spectra correlations virtual screening prediction of active sites library design the prediction of the properties of chemicals the development of new cosmetics products quality control in food the design of new materials with improved properties toxicity modeling assessment of the risk of chemicals and the control of chemical processes The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks Together with the corresponding textbook Chemoinformatics Basic Concepts and Methods ISBN 9783527331093 on the fundamentals of chemoinformatics readers will have a comprehensive overview of the field

Medicinal Chemistry of Nucleic Acids Lihe Zhang, Zhen Xi, Jyoti Chattopadhyaya, 2011-08-10 Complete up to date coverage of the broad area of nucleic acid chemistry and biology Assembling contributions from a collection of authors with expertise in all areas of nucleic acids medicinal chemistry and therapeutic applications Medicinal Chemistry of Nucleic Acids presents a thorough overview of nucleic acid chemistry a rapidly evolving and highly challenging discipline directly responsible for the development of antiviral and antitumor drugs This reliable resource delves into a multitude of subject areas involving the study of nucleic acids such as the new advances in genome sequencing and the processes for creating RNA interference RNAi based drugs to assist pharmaceutical researchers in removing roadblocks that hinder their ability to predict drug efficacy Offering the latest cutting edge science in this growing field Medicinal Chemistry of Nucleic Acids includes In depth coverage of the development and application of modified nucleosides and nucleotides in medicinal chemistry A close look at a large range of current topics on nucleic acid chemistry and biology Essential information on the use of nucleic acid drugs to treat diseases like cancer A thorough exploration of siRNA for RNAi and the regulation of microRNA non coding RNA ncRNA a newly developing and exciting research area Thorough in its approach and promising in its message Medicinal Chemistry of Nucleic Acids probes the new domains of pharmaceutical research and exposes readers to a wealth of new drug discovery opportunities emerging in the dynamic field of nucleic acid chemistry

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