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Special Issue Reprint

Carbohydrate-Based Drugs Discovery

Edited by
Jian Yin, Jing Zeng and De-Cai Xiong

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Carbohydratebased Drug Discovery

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Carbohydratebased Drug Discovery:

Carbohydrate-based Drug Discovery Chi-Huey Wong, 2006-03-06 To exploit the full potential of this diverse compound class for the development of novel active substances this handbook presents the latest knowledge on carbohydrate chemistry and biochemistry While it is unique in covering the entire field particular emphasis is placed on carbohydrates with pharmaceutical potential Topics include the following Chemical Synthesis of Carbohydrates Carbohydrate Biosynthesis and Metabolism Carbohydrate Analysis Cellular Functions of Carbohydrates Development of Carbohydrate based Drugs A premier resource for carbohydrate chemists and drug developers this comprehensive two volume work contains contributions by more than 50 of the world's leading carbohydrate chemists

Carbohydrate-based Drug Discovery, 2 Volume Set Chi-Huey Wong, 2003-10-17 Die Suche nach Medikamenten mit neuen oder verbesserten Eigenschaften hat das Interesse am pharmazeutischen Potenzial von Kohlenhydraten enorm verstärkt Dies gilt insbesondere für die Entwicklung von Antibiotika Impfstoffen und Anti Krebs Mitteln Carbohydrate based Drug Discovery stellt mit mehr als 50 Beiträgen der weltweit führenden Experten die neuesten Entwicklungen in der Kohlenhydrat und Biochemie vor Dabei liegt der Schwerpunkt der Darstellung auf der pharmazeutischen Anwendung In jüngster Zeit sind wirksame auf Kohlenhydraten basierende Medikamente gegen HIV Grippe Epilepsie Diabetes und Krebs auf den Markt gekommen bzw werden in Studien klinisch erprobt Doch das gesamte Potenzial dieser Substanzklasse kann man bislang wohl nur erahnen Die pharmazeutische Industrie investiert bereits große Summen in die Forschung und Entwicklung So kommt dieses Handbuch genau zur richtigen Zeit Umfassend und kompetent behandelt es den gesamten Bereich der Kohlenhydratchemie Es führt ein in die chemische Synthese in Biosynthese und Metabolismus und informiert über die Analyse und die zellulären Funktionen von Kohlenhydraten Einen weiteren Schwerpunkt bildet die Entwicklung von Medikamenten auf Kohlenhydrat Basis wie z B synthetischer Impfstoffe oder Thrombosemittel auf Basis synthetischer Oligosaccharide Erschlossen wird das mit einem umfangreichen bibliographischen Anhang versehene Werk durch einen thematischen Index Sein Herausgeber Chi Huey Wong hat bereits mehrere internationale Preise für sein wissenschaftliches Werk erhalten darunter den Presidential Award und den Presidential Young Investigator Award

Carbohydrates in Drug Discovery and Development Vinod K. Tiwari, 2020-07-31 Carbohydrates in Drug Discovery and Development Synthesis and Applications examines recent and notable developments in the synthesis biology therapeutic and biomedical applications of carbohydrates which is considered to be a highly promising area of research in the field of medicinal chemistry Their role in several important biological processes notably energy storage transport modulation of protein function intercellular adhesion malignant transformation signal transduction viral and bacterial cell surface recognition formulate the carbohydrate systems to be an exceedingly considerable scaffold for the development of new chemical entities of pharmacological importance In addition to their easy accessibility high functionality and chiral pool characteristics are the few additional fascinating structural features of

carbohydrates which further enhance their utilities and thus they have been able to attract chemists and biologists toward harnessing these properties for the past several decades This book covers an advanced aspect of carbohydrate based molecular scaffolding starting with a general introduction followed by a detailed discussion about the impact of diverse carbohydrate containing molecules of great therapeutic values and their impact on drug discovery and development The topics covered in this book include the significance of heparin mimetics as the possible tools for the modulation of biology and therapy chemistry and bioactivities of C glycosylated compounds inositols iminosugars KDO sialic acids glycohybrids macrocycles plant oligosaccharides anti bacterial and anti cancer vaccines antibiotics and more Presents a practical and detailed overview of a wide range of carbohydrate systems including KDO sialic acids inositols iminosugars etc relevant for drug discovery and development Highlights the use of functionalized carbohydrates as synthons for the construction of various systems Covers recent developments in the synthesis of various glycohybrid molecules and vaccines Highlights the significance of heparin mimetics as tools for the modulation of biology Provides an impact of glycan microarrays and carbohydrate protein interaction

Carbohydrates in Drug Design and Discovery Jesus Jimenez-Barbero, F. Javier Canada, Sonsoles Martín-Santamaría, 2015-03-30 In recent years there has been increasing evidence of the importance of carbohydrates and glycoconjugates in biomedical applications and the use of synthetic ligands based on carbohydrates as drugs has received much attention Focussing on drug discovery from key targets and placing an emphasis on the multi disciplinary approaches necessary to challenge these issues this book comprehensively covers the new and recent discoveries in the area of carbohydrate drug discovery Carbohydrates in Drug Design and Discovery is split into five sections beginning with a introduction and perspective on the current market The book then goes on to discuss new synthetic methods in glycobiology the use of glycobiology in chemical biology and glycobiology in drug discovery Providing a worldwide perspective on this broad area and providing examples of therapeutics already developed using these methods this book provides a comprehensive introduction discussion and update on this fast developing field for medicinal chemists and biochemists working in industry and academia

Carbohydrate-Based Drugs Discovery Jian Yin, Jing Zeng, De-Cai Xiong, 2024-03-25 Carbohydrates play an essential role in the organism and have many bioactivities Carbohydrate based drug discovery is an up and coming area of research in medicinal chemistry Bioactive carbohydrates open up a new source for drug development More than 170 carbohydrate based drugs have been successfully approved as anticoagulants antitumor agents antidiabetic agents antibiotics antiviral agents and vaccines However most carbohydrates have low druggability As such new methods and strategies to improve carbohydrates druggability are in high demand This Special Issue aimed to serve as an open forum where researchers can share their experiences and findings on carbohydrate based drugs with a focus on the discovery and development of new carbohydrate based therapeutic agents Contributions to this issue in the form of both original research and review articles cover the separation identification synthesis and pharmacology of bioactive

carbohydrates including monosaccharides oligosaccharides polysaccharides glycopeptides glycoproteins glycomimetics and others *Carbohydrate Chemistry: State Of The Art And Challenges For Drug Development - An Overview On Structure, Biological Roles, Synthetic Methods And Application As Therapeutics* Laura Cipolla,2015-07-23 The structural complexity and the synthetic challenges facing glycans have historically hampered efforts to study their multifaceted roles and the application of carbohydrates in drug development However in very recent years new synthetic techniques flanked by the growing knowledge about carbohydrate involvement in physiological and pathological states has spurred renewed interest in the chemistry biology and therapeutic potentialities of carbohydrates This book offers an overview of key aspects of carbohydrate biology and chemistry that are fundamental for the design of novel therapeutics The four part structure of this book introduces these essential components to life starting from their structure and biological roles and covering analytical methods and synthesis which pave the way for the development of a wide range of therapeutic applications Leading experts from around the world are brought together to offer their recent research with the ultimate aim of enlightening the reader on the complex yet exciting field of carbohydrate chemistry Academic and industrial researchers in structural biology drug discovery and carbohydrate chemistry will find this book an essential guide to the latest research and future potential of medicinal chemistry *Medicinal Chemistry and Drug Discovery: Drug discovery and drug development* Alfred Burger,2003

Studies in Natural Products Chemistry ,2016-09-06 Studies in Natural Products Chemistry Bioactive Natural Products Part XII is the latest in a series that covers the synthesis or testing and recording of the medicinal properties of natural products providing cutting edge accounts of the fascinating developments in the isolation structure elucidation synthesis biosynthesis and pharmacology of a diverse array of bioactive natural products Natural products in the plant and animal kingdom offer a huge diversity of chemical structures that are the result of biosynthetic processes that have been modulated over the millennia through genetic effects With the rapid developments in spectroscopic techniques and accompanying advances in high throughput screening techniques it has become possible to quickly isolate and determine the structures and biological activity of natural products thus opening up exciting opportunities in the field of new drug development to the pharmaceutical industry Focuses on the chemistry of bioactive natural products Contains contributions by leading authorities in the field Presents sources of new pharmacophores **Carbohydrates as Drugs** Peter H. Seeberger,Christoph Rademacher,2014-11-14 Medicinal chemistry is both science and art The science of medicinal chemistry offers mankind one of its best hopes for improving the quality of life The art of medicinal chemistry continues to challenge its practitioners with the need for both intuition and experience to discover new drugs Hence sharing the experience of drug research is uniquely beneficial to the field of medicinal chemistry Drug research requires interdisciplinary team work at the interface between chemistry biology and medicine Therefore the topic related series Topics in Medicinal Chemistry covers all relevant aspects of drug research e g pathobiochemistry of diseases identification and validation of emerging drug targets

structural biology drugability of targets drug design approaches chemogenomics synthetic chemistry including combinatorial methods bioorganic chemistry natural compounds high throughput screening pharmacological in vitro and in vivo investigations drug receptor interactions on the molecular level structure activity relationships drug absorption distribution metabolism elimination toxicology and pharmacogenomics In general special volumes are edited by well known guest editors

Carbohydrate Drug Design Anatoliĭ Alekseevich Klesov, Zbigniew J. Witczak, David Platt, 2006 It is becoming more obvious in recent years that carbohydrates present a new dimension in drug design for targeting specific diseases Carbohydrates birthed a whole new vocabulary into chemistry biochemistry and related disciplines a new language in the form of distinct characters and images providing professional chemists not in the area of carbohydrates to become familiar and knowledgeable on the topic Carbohydrate Drug Design provides the indispensable understanding of the mutual challenge between carbohydrate based drugs and the deadly diseases which they target Carbohydrate Drug Design discusses pre clinical studies and clinical trials of carbohydrate based drugs drug delivery and pain managements biocompatibility clearance and metabolic pathways of carbohydrate drugs and actual medical devices employing carbohydrates The invasion of cancer cells protein glycan interactions and their inhibitors new carbohydrate based therapeutics crystal structure of antibodies with unusually high affinity for carbohydrates and a number of other features of carbohydrate drugs are also comprehensively covered Galactomannans and hyaluronans as well as thio imino and carba sugars are particularly considered in respect to their structural and functional impacts *Carbohydrate-based Synthetic Methodology and Polymer Development* Vishwanath Venkatesh Gaitonde, 2015 Carbohydrates are some of the most abundant organic molecules on earth They are ubiquitous compounds most commonly known for providing energy for working and are biologically stockpiled as glycogen Modern Era advancement in disciplines of glycomics glycobiology and bio renewable studies has played a pivotal role in generating robust interest in the study of carbohydrate chemistry The advances in the field have progressed to cover an expansive range of scientific areas For example there is strong interest in i developing synthetic methodology ii understanding reactivity iii performing structural studies iv exploring enzyme catalysis v biological and medical applications as well as exploiting their use in food and polymer industries From a biological perspective it is recognized that carbohydrates play a fundamental role in cell recognition cell cell interaction cell differentiation cell growth survival of living cells and organisms Synthetically a variety of natural products and antibiotics contains carbohydrate moieties providing a vast platform for glyco based synthesis In addition biochemical inquiries over last few decades have established the association of carbohydrates with various disease conditions and identified glycans as untapped tools in drug discovery Development of the carbohydrate based drug discovery can be categorized by one of the following approaches i producing native glycans with desired biological activity ii structural modification via glycomimetic approaches iii generating a glyco scaffold for achieving carbohydrate diversity and iv developing glyco fused therapeutics The scope of work covered in this

dissertation covers several carbohydrate related areas First we desired to i develop a series of glycosyl amide linkages demonstrating the use of glycosyl 2 4 dinitrobenzenesulfonamides as key intermediates in the chemoselective formation of these motifs ii produce glycosyl fluoride moieties to study their potential inhibitory activity against Mycobacterium tuberculosis Mtb GlgE iii generate oligosaccharides to study their interaction with the glucan binding site of Mtb GlgE and iv demonstrate the utilization of furfural degradation product of pentose sugars from hemicellulose bio resource to access a bisfuran monomer in order to generate furan based polymeric materials Glycosyl amide linkages are key motifs found in glycosyl amino acids N linked glycopeptides besides several natural products Some of the popular strategies to access these linkages include Lansbury aspartylation involving direct coupling of glycosylamine with activated aspartic acid on protected amino acid Alternatively a route to access glycosyl amide linkage is via Staudinger reduction acylation or traceless Staudinger ligation of glycosyl azide This method ends up producing a mixture of a glycosyl amides 2 4 Dinitrobenzenesulfonyl chloride dNBS Cl has been used to protect the primary amines producing the 2 4 dinitrobenzenesulfonamides dNBS NH₂ dNBS dNBS can be used to produce secondary amines and diamines as noted by Fukuyama et al dNBS were later explored for producing amides thioamides ureas and thioureas and only very recently this strategy has been taken as a possible chemoselective approach to form peptide linkage and neoglycoconjugates To further this chemistry in our chemoselective studies producing the glycosyl amides we explored the scope of this methodology by reacting a series of dNBS glycosides with thioacetic acid The N glycosyl 2 4 dinitrobenzenesulfonamides were accessed via benzoyl protected glycosyl azides The azides were i reduced with Adams catalyst to the corresponding amines ii the glycosylamines were sulfonated with 2 4 dinitrobenzenesulfonyl chloride to form N glycosyl 2 4 dinitrobenzenesulfonamides in moderate yields and iii the glycosyl amides were then prepared in 67 81 % yields by treatment of the sulfonamides with thioacetic acid and cesium carbonate The conversion of the glycosylsulfonamide to the glycosyl amide proceeded with high stereoselectivity A second project area involved new approaches to preprepare oligosaccharide Mtb is the causative agent of tuberculosis TB which is one of the leading cause of death due to an infectious disease Designing substrates inhibitors and biochemical probes to understand and overcome this disease condition is of significant interest Mtb GlgE an a 1 4 glucan phosphate maltosyltransferase is a genetically validated tuberculosis target Underlining this target we designed glycosyl fluoride derivatives as biochemical probes to determine the active site residues and better understand the Mtb GlgE catalytic mechanism 5 fluoro L idosyl fluoride an epimer of 5 fluoro D glucosyl fluoride has been synthesized over 5 steps Starting with D glucose a key step was photobromination at the C 5 using NBS and AIBN followed by substituting the bromide with fluoride using AgF Mtb GlgE transfers the maltosyl units on to the elongating the a 1 4 glucan polymer As a concurrent project we sought to access the oligosaccharide units mimicking the a glucan polymer in the Mtb GlgE The oligosaccharides are envisioned to be useful for probing the a glucan binding site During the oligosaccharide synthesis we propose a

stereoselective glycosylation strategy was pursued applying a preactivation methodology Starting with D maltose the building blocks for the a 1 4 glucan oligosaccharide were accessed via a divergent synthetic route by creating the donor 4 6 O benzylidene maltosyl thioglycoside and the acceptor 4 OH maltosyl thioglycoside substrates During synthesis the donor is first accessed which was further regioselectively reduced at the 4 6 O benzylidene to create 4 OH non reducing end generating the acceptor substrate Glycosylation between the donor and acceptor substrate is then envisioned to proceed using a 2 2 preactivated method to build the tetrasaccharide unit This tetrasaccharide on regioselective reduction at the 4 6 O benzylidene creates the 4 OH non reducing end which then acts as a template to produce 4 2 hexasaccharide and or 4 4 octasaccharide and so on to access a 1 4 glucan oligosaccharide units of desired length In a final area of research carbohydrates were explored as feedstocks for polymer synthesis Starch is commonly understood as a first generation biorenewable feedstock and lignocellulose as second generation biorenewable Lignocellulose consists of cellulose 40 45 % hemicellulose 24 40 % and lignin 18 25 % Hemicellulose consists chiefly of the pentose sugar xylose and arabinose The degradation of these pentose sugars yields furfural The latter is considered to be a leading candidate for bio renewable building blocks and as a platform chemical for its application in diverse commercial sectors In the same direction there is a substantial interest and progress in the utilization of this bio based feedstock to fulfill the growing demands in the sector of fuel chemical pharmaceutical and polymer industries As a part of our preliminary investigation starting with commercial furfural we have designed a four steps synthetic route to access a bisfuran diol BFD as a monomer feedstock to generate polymeric materials Starting with commercial furfural i reaction with 1 2 ethanedithiol in recyclable glycerol produced the 1 3 dithiane protected furfural in 93 % yield after distillation ii treatment with acetone and 50% aqueous sulfuric acid produced a dimerized Friedel Crafts product in 58% yield iii deprotection of the 1 3 dithiane was accomplished using selenium dioxide along with acetic acid to generate dialdehyde in 90% yield and iv the penultimate dialdehyde was reduced to afford the final diol the BFD in 96 % yield BFD was crystallized in the monoclinic space group and X ray studies were undertaken to understand the molecular arrangement in space hydrogen bonding and packing of the molecule These set of data were compared with Bisphenol A BPA a known endocrine disruptor and its known derivatives to predict the potential estrogenic or anti estrogenic activities in BFD Further BFD was employed in polymerization studies to successfully generate bisfuran polyester BFPE 1 a low molecular weight novel polyester material of amorphous nature

Carbohydrate-Based Therapeutics Roberto Adamo, Luigi Lay, 2023-08-28 Carbohydrate Based Therapeutics Comprehensive resource summarizing opportunities and latest progress in design methodologies for carbohydrate based therapeutics through a disease oriented approach Carbohydrate Based Therapeutics covers current progress and explores new frontiers in carbohydrate based therapeutic applications utilizing a unique approach by providing a detailed background of diseases coupled with subsequent carbohydrate based therapies The link between chemistry and design of novel carbohydrate based medicines is highlighted

and a broad overview of all the potential applications of carbohydrates is given. Emphasis is laid on concepts used for carbohydrate drug design, structure-activity relationship, and impact on health and diseases. The text also discusses newer topics like nanoparticles, material science, and tissue generation. Carbohydrate Based Therapeutics includes information on antimicrobial carbohydrate based therapies covering antibacterial and antiviral vaccines, antifungal therapies, anti-influenza therapeutics, and antiadhesive carbohydrates and glycomimetics. Anti-cancer carbohydrate based therapies covering cancer vaccines and immunotherapy, and carbohydrate tools in cancer biology. Carbohydrate based therapies in metabolic, neuronal, and immune disorders covering carbohydrate based therapeutics for lysosomal disorders and neurodegenerative diseases. New frontiers in carbohydrate based therapies covering carbohydrates for tissue engineering, antiangiogenic, and regenerative medicine. Providing comprehensive coverage of foundational knowledge on the subject in a unique and highly accessible format while also exploring the state of the art in the field's applications. Carbohydrate Based Therapeutics is an essential resource for medicinal, pharmaceutical, and organic chemists, chemists in industry, biochemists, and biotechnologists.

Combinatorial Chemistry and Molecular Diversity in Drug Discovery Eric M. Gordon, James F. Kerwin, 1998-08-27

Increasing pressure to identify, optimize, develop, and commercialize novel drugs more rapidly and more cost effectively has led to an urgent demand for technologies that can reduce the time to market for new products. Molecular diversity of both natural and synthetic materials provides a valuable source of compounds for identifying and optimizing new drug leads. Through the rapidly evolving technology of combinatorial chemistry, it is now possible to produce libraries of small molecules to screen for novel bioactivities. This powerful new technology has begun to help pharmaceutical companies find new drug candidates quickly, save significant dollars in preclinical development costs, and ultimately change their fundamental approach to drug discovery. Included among the many topics: Historical background, Library strategy and design, Solid phase synthesis, Small molecular libraries, Automation, analytical and computational methodology, Biological diversity, Strategies for screening combinatorial libraries, Combinatorial drug screening and development, Combinatorial chemistry information management.

Medicinal Chemistry and Drug Discovery: Nervous system agents Alfred Burger, 2003 *Burger's Medicinal Chemistry and Drug Discovery, Principles and Practice* Alfred Burger, Manfred E. Wolff, 1995-01-02 **BURGER'S MEDICINAL CHEMISTRY AND DRUG DISCOVERY FIFTH EDITION Volume 1 Principles and Practice** This new edition of Dr Alfred Burger's internationally celebrated classic helps researchers acquaint themselves with both traditional and state of the art principles and practices governing new drug research and development. Completely updated and revised to reflect the many monumental changes that have occurred over the past decade and a half in medicinal chemistry and new drug development, this latest edition of Volume 1 Principles and Practice now covers the latest methods of drug discovery, including such hot topics as computational chemistry and peptidomimetics. Has added emphasis on preclinical development issues. Offers the most timely information on a broad range of important regulatory, management, legal, and financial issues.

Features in depth coverage of important factors in the discovery process including ADME toxicity and drug allergy and clinical trials Updates readers on recent advances in the understanding of the structural biology of drug action Explores the cutting edge technologies for drug discovery now in use around the world Is more than twice the size of its predecessor Brings together contributions by experts in a wide range of related fields from North America and Europe

Carbohydrate-Based Vaccines and Immunotherapies Zhongwu Guo,Geert-Jan Boons,2009-06-09 The fundamental science and the latest developments in carbohydrate based vaccines The relatively new field of glycoimmunology has emerged from the marriage of glycobiology and immunology in recognition of the important role carbohydrates play as antigenic determinants Carbohydrate Based Vaccines and Immunotherapies comprehensively reviews the state of this exciting field offering a single source for both the fundamental science and the latest developments With contributions by leading experts this resource covers the design synthesis evaluation and applications of various carbohydrate based vaccines including polysaccharides neoglycoproteins and neoglycolipids The text approaches vaccine design from a chemical and molecular focus staying in line with current advances Key topics covered by Carbohydrate Based Vaccines and Immunotherapies include Recent developments towards clinically useful vaccines against bacteria viruses parasites and fungi Using adjuvants to improve immunogenicity and or immunological properties of vaccines Choosing and designing proper adjuvants for specific targets Abnormal carbohydrates expressed by tumors Carbohydrate based therapeutic cancer vaccines or cancer immunotherapy Clinical trials results for synthetic cancer vaccines Glycoengineering of cell surface carbohydrates and its anticancer applications Using cell surface carbohydrates for disease diagnosis A single convenient source of state of the art information from leading authorities in the field Carbohydrate Based Vaccines and Immunotherapies is an essential reference for organic chemists and biochemists academic researchers and other students and professionals involved in vaccine design Journal of Scientific and Industrial Research ,2001 **Inorganic Nanomedicine: Synthesis,**

Characterization and Application Amir Al-Ahmed,Arun M. Isloor,M. Nasiruzzaman Shaikh,2013-04-24 Special topic volume with invited peer reviewed papers only **Ligand-Macromolecular Interactions in Drug Discovery** Ana Cecília A. Roque,2010-03-23 In this authoritative book experts in the field highlight the main principles and methodologies currently utilized in the study of molecular interactions between compounds This is as an ideal guide to those striving to further our knowledge of medicines **Advances Towards Synthesis of C-glycosyl Tumor-associated Carbohydrate Antigens** Christopher Arthur LeClair,2006

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