



RSC Drug Discovery

# Carbohydrates in Drug Design and Discovery

Edited by Jesus Jimenez-Barbero, F. Javier Canada  
and Sonsoles Martin-Santamaria



# Carbohydrates In Drug Design

**Zbigniew Witczak**



## **Carbohydrates In Drug Design:**

**Carbohydrates in Drug Design and Discovery** Jesús Jiménez-Barbero, F. Javier Cañada, Sonsoles

Martin-Santamaría, 2015-04-10 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 an 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 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.

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 chiralpool 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

*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 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      **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-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 Thrombosedmittel 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 Design Zbigniew Witczak, 1997-06-11 Emphasizes the role of carbohydrates as anti inflammatory anticancer antidiabetic anticonvulsant antibiotic and antiviral agents The text covers chemical properties biological functions methodologies for synthesizing model compounds conformational and steric effects synthetic and enzymatic approaches and the discovery and development of leads in emerging fields      *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

**Current Medicinal Chemistry**, 1999-02 *Microbial Glycobiology* Anthony P Moran, 2009-10-01 This book presents in an easy to read format a summary of the important central aspects of microbial glycobiology i e the study of carbohydrates as related to the biology of microorganisms Microbial glycobiology represents a multidisciplinary and emerging area with implications for a range of basic and applied research fields as well as having industrial medical and biotechnological implications Individual chapters provided by leading international scientists in the field yield insightful concise and stimulating reviews Provides researchers with an overview and synthesis of the latest research Each chapter begins with a brief 200 word Summary Abstract detailing the topic and focus of the chapter as well as the concepts to be addressed Allows researchers to see at a glance what each chapter will cover Each chapter includes a Research Focus Box Identifies important problems that still need to be solved and areas that require further investigation

*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

Comprehensive Medicinal Chemistry III ,2017-06-03 Comprehensive Medicinal Chemistry III Eight Volume Set provides a contemporary and forward looking critical analysis and summary of recent developments emerging trends and recently identified new areas where medicinal chemistry is having an impact The discipline of medicinal chemistry continues to evolve as it adapts to new opportunities and strives to solve new challenges These include drug targeting biomolecular therapeutics development of chemical biology tools data collection and analysis in silico models as predictors for biological properties identification and validation of new targets approaches to quantify target engagement new methods for synthesis of drug candidates such as green chemistry development of novel scaffolds for drug discovery and the role of regulatory agencies in drug discovery Reviews the strategies technologies principles and applications of modern medicinal chemistry Provides a global and current perspective of today s drug discovery process and discusses the major therapeutic classes and targets Includes a unique collection of case studies and personal essays reviewing the discovery and development of key drugs

The Science and Business of Drug Discovery Edward D. Zanders,2020-11-09 The Science and Business of Drug Discovery is written for those who want to learn about the biopharmaceutical industry and its products whatever their level of technical knowledge Its aim is to demystify the jargon used in drug development but in a way that avoids over simplification and the resulting loss of key information Each of the twenty chapters is illustrated with figures and tables which clarify some of the more technical points being made Also included is a drug discovery case history which draws the relevant material together into a single chapter In recognizing that it is difficult to navigate through the many external resources dealing with drug development the book has been written to guide the reader towards the most appropriate information sources including those listed in the two appendices The following topics are covered Different types of drugs from small molecules to stem cells Background to chemistry of small and large molecules Historical background to drug discovery pharmacology and biotechnology The drug discovery pipeline from target discovery to marketed medicine Commercial aspects of drug discovery Challenges to the biopharmaceutical industry and its responses Material of specific interest to technology transfer executives recruiters and pharmaceutical translators Essentials of Carbohydrate Chemistry and Biochemistry Thisbe K.

Lindhorst,2007-04-09 Concise yet complete this is a succinct introduction to the topic covering both basic chemistry as well as such advanced topics as high throughput analytics and glycomics in one handy volume This improved and expanded 3rd edition features all new material on combinatorial synthesis of carbohydrates and carbohydrate biodiversity and each chapter now contains study questions for self learning and classroom teaching Didactically written by an experienced lecturer and

graduate student advisor the text is backed by practical examples and more than 150 study questions tailored to students needs

*Carbohydrate Mimics* Yves Chapleur,1998-09-10 Carbohydrate Mimics Concepts and Methods Edited by Yves Chapleur Apart from the various functions of carbohydrates in natural processes they are important building blocks for drugs especially antibiotics In addition carbohydrates are considered as important structures in the immunological recognition process of the antigen antibody reaction The modification of the structure and thereby the chemistry of substrates is a common procedure in nature This naturally occurring process is reflected in the concept of molecular mimicry which has become a useful approach in drug discovery The search for carbohydrate analogues that exhibit better binding activity biological activity and stability began with the synthesis of azasugars A lot of structural modifications around the anomeric center of carbohydrates has been achieved over the last decade and these are summarized in terms of the different chemical and biological aspects of carbohydrate mimics in one part of this book In addition to the well established fields of C glycosides azasugars and carbasugars the other part of the book focusses on outstanding achievements in carbohydrate mimic research Everybody who is active in carbohydrate research or is interested in moving into this exciting field will benefit from this up to date source of informations The leading experts in this field describe their scientific approaches to real interdisciplinary puzzles This book should be an inspiration to scientists in organic medicinal chemistry biochemistry and biology

**Pharmacognosy** Simone Badal McCreath,Yuri N. Clement,2023-10-13 Pharmacognosy Fundamentals Applications and Strategies Second Edition represents a comprehensive compilation of the philosophical scientific and technological aspects of contemporary pharmacognosy The book examines the impact of the advanced techniques of pharmacognosy on improving the quality safety and effectiveness of traditional medicines and how pharmacokinetics and pharmacodynamics have a crucial role to play in discerning the relationships of active metabolites to bioavailability and function at the active sites as well as the metabolism of plant constituents Structured in seven parts the book covers the foundational aspects of Pharmacognosy the chemistry of plant metabolites their effects other sources of metabolites crude drugs from animals basic animal anatomy and physiology technological applications and biotechnology and the current trends in research New to this edition is a chapter on plant metabolites and SARS Cov 2 extensive updates on existing chapters and the development of a Laboratory Guide to support instructors execute practical activities on the laboratory setting Covers the main sources of natural bioactive substances Contains practice questions and laboratory exercises at the end of every chapter to test learning and retention Describes how pharmacokinetics and pharmacodynamics play a crucial role in discerning the relationships of active metabolites to bioavailability and function at active sites Includes a dedicated chapter on the effect of plant metabolites on SARS CoV 2

**Medicinal Chemistry and Drug Discovery: Drug discovery and drug development** Alfred Burger,2003 **The Design, Synthesis and Evaluation of New Chemical Entities for the Development of Drugs Against Cancer, Diabetes, Autoimmune Disorders and Infectious Diseases** Li Gao,2004

New Perspectives in Drug Design Philip Michael Dean, Georges Jolles, C. G. Newton, 1995 This text updates the first Rhone Poulenc Rorer Round Table Conference volume on the subject of drug design It covers topics from the practicalities of synthetic organic chemistry to the potential pitfalls in the mathematics of free energy calculations

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