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Bioisosteric Approach and Drug Design

First Edition

Editor

Dr. Sanmati Kumar Jain

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Bioisosteric Approach and Drug Design

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Table of Contents

Chapter No.	Contents	Page No.
1	Bioisosteric Approach: A Brief Introduction and Historical Perspective <i>Sanmati Kumar Jain</i>	1-16
2	Classical Bioisosteres: A Rational Approach in Drug Design <i>Aashif Khan and Sanmati K. Jain</i>	17-28
3	Non-Classical Bioisosteres <i>Sanmati Kumar Jain</i>	29-63
4	Bioisosteric Approach and Metabolic Stability <i>Achal Mishra and Sanmati K. Jain</i>	64-70
5	Bioisosteric Approach in Potency Improvement and Toxicity Reduction <i>Sanmati Kumar Jain</i>	71-92
6	Bioisosteric Approach and Bioavailability <i>Yogesh Vaishnav and Sanmati Kumar Jain</i>	93-102
7	Bioisosteres of Amide: A Case Study With Pemetrexed, An Anti-Folate Cytostatic Agent <i>Ajay Kumar Gupta and Sanmati Kumar Jain</i>	103-124
8	Bioisosteres of Amine: A Case Study With Cytarabine, An Antineoplastic Agent <i>Ajay Kumar Gupta and Sanmati Kumar Jain</i>	125-144
9	Bioisosteres of Bipyridine: A Case Study With Etoricoxib, A Cyclooxygenase-2 Inhibitor <i>Girija Prasad Swain, Ajay Kumar Gupta, Achal Mishra and Sanmati Kumar Jain</i>	145-159
10	Bioisosteres of Carboxylic Acid: A Case Study With Aceclofenac, A Nonsteroidal Anti-Inflammatory Drug <i>Dipti Pal and Sanmati K. Jain</i>	160-182
11	Bioisosteres of Catechol Functional Group <i>Anjali Suryavanshi, Yugal Kishor Shukla, Pragya Gupta, Vandana, Karthikeyan Kesavan and Sanjay Kumar Bharti</i>	183-197
12	Bioisosteres of Guanidine Functional Group <i>Vandana, Yugal Kishor Shukla, Anjali Suryavanshi, Pragya Gupta, Karthikeyan</i>	198-213

	<i>Kesavan and Sanjay Kumar Bharti</i>	
13	Bioisosteres of Halogen Group <i>Dipti Pal and Sanmati Kumar Jain</i>	214-236
14	Bioisosteres of Hydroxy Group: A Case of Paracetamol as Non-Steroidal Anti-Inflammatory Drugs (NSAIDS) <i>Dipti Pal and Sanmati Kumar Jain</i>	237-256
15	Bioisosteres of Phenyl Group: Reported Bioisosteres and A Case Study With Diclofenac, A Preferential Cyclooxygenase-2 Inhibitor <i>Girija Prasad Swain, Ajay Kumar Gupta, Sanjay Kumar Lanjhiyana and Sanmati Kumar Jain</i>	257-278
16	Bioisosteres of Phenoxy Group: A Case Study With Rosiglitazone as PPAR-γ Activator in Diabetes Mellitus Treatment <i>Aashif Khan and Sanmati K. Jain</i>	279-292
17	Bioisosteres of Pyridine: A Case Study With Palbociclib, A Cyclin-Dependent Kinase Inhibitor <i>Ajay Kumar Gupta, Gajendra Singh Thakur and Sanmati Kumar Jain</i>	293-312
18	Bioisosteres of Quinoline-4-oxy: A Case Study With Cabozantinib, Tyrosine Kinase Inhibitors <i>Gajendra Singh Thakur, Ajay Kumar Gupta, Neeraj Kumar and Sanmati Kumar Jain</i>	313-325
19	Bioisosters of Urea and Thiourea <i>Mohammad Akbar Siddiqui, Sakshi Gupta, S. K. Lanjhiyana, Meenakshi Jaiswal, Sweety Lanjhiyana, Sanmati Kumar Jain and Nidhi Agrawal</i>	326-340
20	Bioisosteres of Carbamate: A Case Study With Rivastigmine, An Acetylcholinesterase Inhibitor in Alzheimer's Disease Treatment <i>Yogita Sahu and Sanmati K. Jain</i>	341-356
21	Design of Pyrazole Bioisoesters: A Case Study With Remogliflozin Etabonate as Sglt-2 Inhibitors in Anti-Diabetic Therapy <i>Ritu Soni, Ajay Kumar Gupta, Yogesh Vaishnav and Sanmati Kumar Jain</i>	357-379

22	Bioisosteres of Sulfonamide: A Case Study With Furosemide, Sodium-Potassium-Chloride Cotransporter Inhibitor <i>Ritu Soni, Ajay Kumar Gupta and Sanmati Kumar Jain</i>	380-399
23	Bioisosteres of Carbonyl Group: A Case Study With Megestrol, As An Anticancer Drug <i>Yogesh Vaishnav, Ajay Kumar Gupta, Dipti Pal and Sanmati Kumar Jain</i>	400-419

Preface

Bioisosteres are substituents or groups that provide comparable biological properties based on similar chemical or physical properties. A common feature in drug design is bioisosterism, which has led to the development of newer analogues with greater potency, reduced toxicity, better pharmacokinetics, improved selectivity, and increased metabolic stability. The fundamental idea of bioisosterism is that molecules with dissimilar structures can yet have comparable biological functions provided they have certain essential physicochemical characteristics in common. The aim is to strategically alter a medication molecule's structure in order to maximize the ratio between safety and effectiveness.

In the field of drug discovery, where creativity is crucial, bioisosterism plays a vital role in innovative molecular design. It is a principle based on the deep realization that slight alterations in chemical structure can result in significant variations in biological effects. This book explores the complex realm of bioisosterism, a journey that crosses the boundaries of chemistry, biology, and pharmacology.

Bioisosterism is a useful technique for medicinal chemists, enabling the replacement of functional groups or atoms with others that possess similar biological properties. By systematically investigating and designing bioisosteres, opportunities arise to enhance drug potency, refine pharmacokinetics, and minimize adverse effects. This document provides an in-depth examination of the principles and practical applications of bioisosterism in drug development.

The book provides an extensive examination of bioisosterism, encompassing its historical perspective, classical and non-classical bioisosteres, and approaches to improve drug molecules by augmenting metabolic stability, potency, minimizing side effects and toxicity, and optimizing bioavailability.

This book covers a wide range of bioisosteres, including amide, bipyridine, carboxylic acid, catechol, guanidine, halogen, hydroxyl, phenyl, phenoxy, pyridine, quinoline-4-oxy, urea, carbamate, pyrazole, sulfonamide, and carbonyl groups, and their applications in drug design. By presenting case studies involving different functional groups in diverse therapeutic areas, from antibiotics, anti-inflammatory drugs, anti-diabetic medications, diuretics to anticancer agents, the book highlights the importance of bioisosteres in enhancing drug efficacy and safety.

My profound gratitude goes out to Dr. M. Prakash of Excellent Publishers for their unwavering support and gracious collaboration in bringing forth this edition in an expedited manner.

As authors deeply immersed in the field, our primary objective is to offer a

comprehensive guide that caters to a wide range of individuals, including seasoned researchers, professionals, curious students (Chemistry, Pharmacy, Pharmaceutical Chemistry, Medicinal Chemistry), as well as those who are new to the subject or simply have a keen interest in scientific exploration. This book serves as an all-encompassing resource for understanding and harnessing the potential of bioisosterism. We extend a warm invitation for you to accompany us on this intellectual journey, where scientific inquiry converges with practical application, and where the pursuit of better medicines drives innovation and discovery. May it ignite your curiosity about the molecules that shape our world and inspire you to envision the possibilities that lie ahead in the pursuit of a healthier future.

Any recommendations aimed at increasing the book's value will be gratefully reviewed for inclusion in upcoming editions.

Sanmati Kumar Jain

About the Editor



Dr. Sanmati Kumar Jain is an esteemed Professor of Pharmaceutical Chemistry at Guru Ghasidas Vishwavidyalaya (A Central University) Bilaspur, India. With a remarkable teaching career spanning twenty-three years at both postgraduate and undergraduate levels, he has established himself as a highly experienced educator. Dr. Jain's contributions to the field of pharmaceutical chemistry are evident through his publication of more than eighty research papers in prestigious national and international scientific journals. His guidance has been instrumental in the successful completion of 30 M. Pharm. and 3 Ph.D. degrees.

Recognized for his outstanding research work, Dr. Jain has been honoured with the Best Research Paper Award and Best Researcher award. His expertise is further demonstrated by his authorship of over 80 scientific articles in reputable journals and his contribution to 32 book chapters. Additionally, he has presented more than 30 research works at various national and international conferences and seminars.

Dr. Jain's research endeavours have been supported by a research project funded by AICTE-RPS. He has also authored a book and holds 21 patents, with 9 granted and 12 published. His research interests primarily lie in the field of Drug Design and Medicinal Chemistry.

As a dedicated professional, Dr. Jain is an active life member of esteemed organizations such as the Indian Pharmaceutical Association (IPA), Association of Pharmaceutical Teachers of India (APTI), and Society of Pharmaceutical Education and Research (SPER). Furthermore, he serves as a reviewer for numerous peer-reviewed international journals, contributing to the advancement of scientific knowledge in his field.