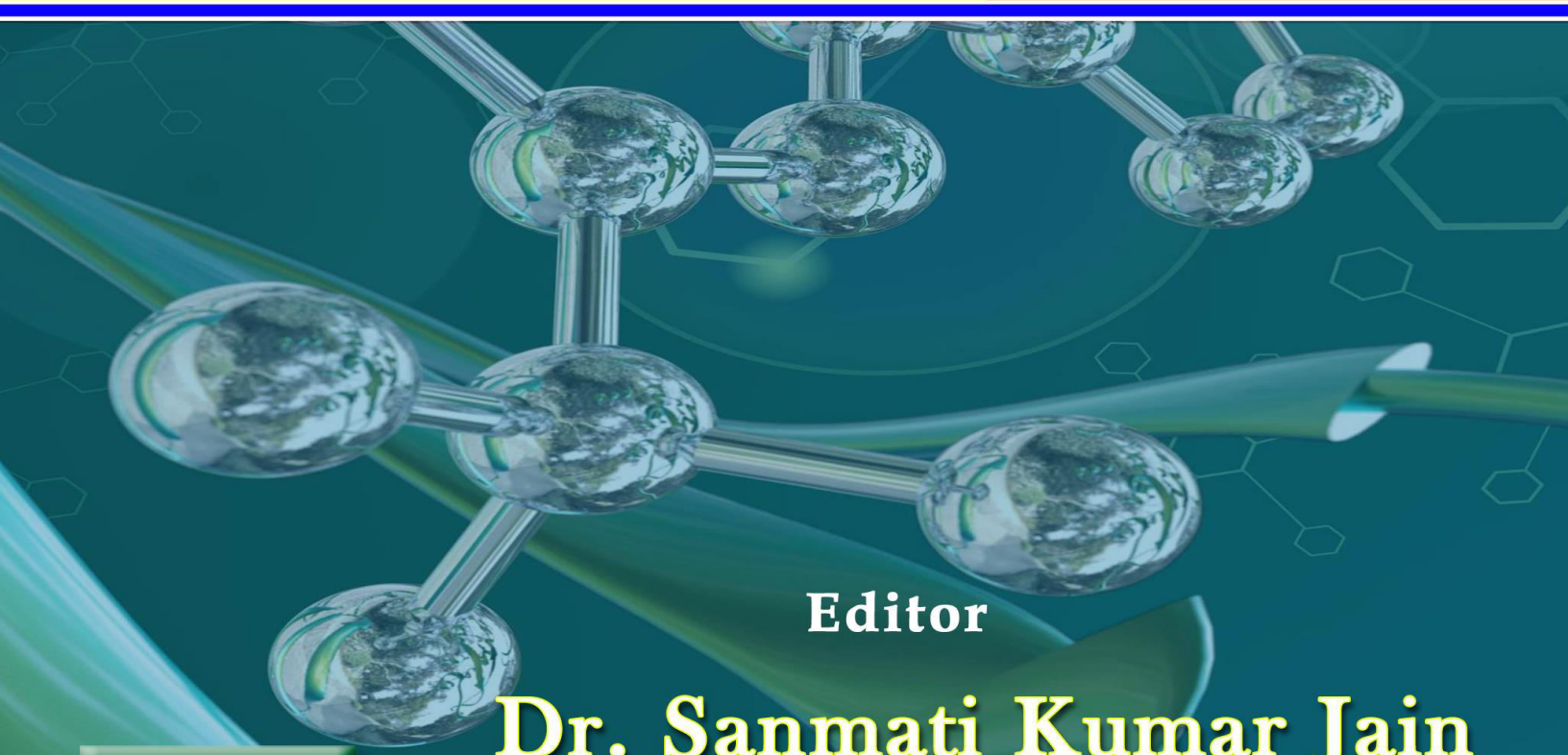
ISBN-978-93-94174-48-1

Bioisosteric Approach and Drug Design

First Edition



Editor

Dr. Sanmati Kumar Jain

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Bioisosteric Approach and Drug Design

Editor

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Publication Date: 30-06-2024

ISBN: 978-93-94174-48-1

https://doi.org/10.20546/ 978-93-94174-48-1

Excellent Publishers

Excellent Publishers
Kancheepuram, India
www.excellentpublishers.com
email id: excellentpublishers2013@gmail.com

Publisher: **Excellent Publishers**
Editor: **Dr.Sanmati Kumar Jain,**
ISBN: 978-93-94174-48-1
https://doi.org/10.20546/ 978-93-94174-48-1

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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 GhasidasVishwavidyalaya (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.