Medicinal and Environmental Chemistry: Experimental Advances and Simulations

PART 1

Editors:

Tahmeena Khan
Abdul Rahman Khan
Saman Raza
Iqbal Azad
Alfred J. Lawrence

Bentham Books

Medicinal and Environmental Chemistry: Experimental Advances and Simulations (Part I)

Edited by

Tahmeena Khan
Integral University
Department of Chemistry
India

Abdul Rahman Khan
Integral University
Department of Chemistry
India

Saman Raza
Isabella Thoburn College
Department of Chemistry
India

Iqbal Azad
Integral University
Department of Chemistry
India

&

Alfred J. Lawrence
Isabella Thoburn College
Department of Chemistry
India

Medicinal and Environmental Chemistry:
Experimental Advances and Simulations *(Part I)*

Editors: Tahmeena Khan, Abdul Rahman Khan, Saman Raza, Iqbal Azad and Alfred J. Lawrence

ISBN (Online): 978-981-4998-27-7

ISBN (Print): 978-981-4998-28-4

ISBN (Paperback): 978-981-4998-29-1

need for a court order if at any point you breach any terms of this License Agreement. In no event will any delay or failure by Bentham Science Publishers in enforcing your compliance with this License Agreement constitute a waiver of any of its rights.

3. You acknowledge that you have read this License Agreement, and agree to be bound by its terms and conditions. To the extent that any other terms and conditions presented on any website of Bentham Science Publishers conflict with, or are inconsistent with, the terms and conditions set out in this License Agreement, you acknowledge that the terms and conditions set out in this License Agreement shall prevail.

Bentham Science Publishers Pte. Ltd.
80 Robinson Road #02-00
Singapore 068898
Singapore
Email: subscriptions@benthamscience.net

CONTENTS

FOREWORD

Environmental pollution (air, water and soil) and human health are inextricably linked. The developing countries are engaged in a wide range of activities that are causing enormous damage to the environment, ecosystems that sustain both our species and Earth's legacy of biodiversity, and human health. If our society takes constructive actions now, or at least soon, it will not be too late to prevent or repair many of these important environmental problems, which threaten the welfare of people and most other species. A more respectful attitude toward the natural world is also urgently needed, for the world is one family, "Vasudhaiva Kutumbakam".

This innovative book will attract scientists interested in environmental pollution and human health with a view to offer remediation techniques. The book chapters have been authored by experts from their fields, both scientists and academicians, and would benefit the readers.

Viney P. Aneja
North Carolina State University
USA

PREFACE

With the drastic disturbance in environmental harmony and balance, there has been a rise in global deaths and diseases, calling for the exploration of novel remediation strategies for innovative drug action mechanisms and target identification. The fine balance between human and ecological health is getting disturbed, leading to serious implications, including the occurrence of new pathogens and diseases, the novel coronavirus SARS-CoV-2, being the most recent instance having gripped the entire globe.

Environmental diseases are non-communicable and are caused by chronic exposure to toxic pollutants. Other contributory causes of environmental diseases include radiation, pathogens, allergens and psychological stress. Their increasing occurrence is due to industrialization, changes in farming protocols and the increase in exposure to chemicals released into the environment. Lifestyle changes, including the increased use of tobacco and processed foods, also greatly contribute to the environmental/lifestyle diseases burden.

Though separately medicinal chemistry and environmental chemistry have been widely explored, yet their close association and interdependence have been overlooked. By exploring the association between these two focal areas, the present book aims to provide solutions and curative strategies for the well-being of humans and the environment as a whole.

The ten chapters included in this book are focused on diverse topics trying to blend the fields of environmental chemistry and medicinal chemistry and have been authored by experts, scientists and academicians from renowned institutions. A wide range of topics has been explored in the book to make it relevant to environmental chemists and students. The chapters have been designed so as to introduce environmental contaminants and techniques for their quantification and removal. Also, a medicinal perspective for remediation of environmental hazards, from therapeutic strategies available to the design of new and safer drugs, is introduced through experimental and simulation approaches.

Specialized chapters have been dedicated to persistent organic pollutants, heavy metals, and plastics, which have become a major source of pollution, along with their remediation. The effect of environmental xenoesterogens on human health has been discussed in one chapter, while in another, the potential of natural curing agents to combat ecotoxicity has been explored. To further elaborate the importance of safe chemical practice, the concept of green chemistry has also been introduced.

As we are aware that drug discovery for a particular disease is a time taking endeavour, therefore a few chapters have also been dedicated to in-silico predictions like molecular docking and virtual models for biological properties, the software used and their utility in making futuristic and accurate predictions to make drug discovery efficient, quicker and cost-effective. Chapters summarizing the challenges of medicinal chemistry as well as the advances of biomolecular simulations for drug designing with respect to ecotoxicity are also included.

The book will prove beneficial for academicians, students of environmental chemistry, pharmacy, researchers, scientists, computational chemists, pharmacologists, environmentalists, policymakers and postgraduate students. It would also provide researchers and medicinal chemists the information regarding the latest research done and the modern techniques used to develop more effective and safer drugs that would not be harmful to the environment. In this way, the proposed book would be highly beneficial to the audience it hopes to cater to.

Tahmeena Khan
Integral University
Department of Chemistry
India

Abdul Rahman Khan
Integral University
Department of Chemistry
India

Saman Raza
Isabella Thoburn College
Department of Chemistry
India

Iqbal Azad
Integral University
Department of Chemistry
India

&

Alfred J. Lawrence
Isabella Thoburn College
Department of Chemistry
India

List of Contributors

Ahmad I.	Isabella Thoburn College, Lucknow, India
Ahmad M.	Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, India
Alam Z.	Shibli National PG College, Azamgarh, India
Ali A.	Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, India
Ansari J.A.	King George's Medical University, Lucknow, India Shibli National PG College, Azamgarh, India
Azad I.	Integral University, Lucknow, India
Bajpai S.	Amity University, Lucknow, India
Bhatia S.	Isabella Thoburn College, Lucknow, India
Bhatia S.	Isabella Thoburn College, Lucknow, India
Biswas K.	Indian Institute of Technology Kanpur, Kanpur, India
Gupta A.	CSIR-Central Institute of Medicinal and Aromatic Plants (CSIR-CIMAP), Lucknow, India
Gupta N.	CSIR-Indian Institute of Toxicology Research, Lucknow, India
Jabeen F.	Jazan University, Jazan, Saudi Arabia
Khan A. R.	Integral University, Lucknow, India
Khan M.A.	K.K.L.K.M, Kathara, Kanpur, India
Khan T.	Integral University, Lucknow, India
Khare A.	Indian Institute of Technology Kanpur, Kanpur, India
Kumar S.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Mahdi A. A.	King George's Medical University, Lucknow, India
Mishra A.	Indian Institute of Information Technology, Prayagraj, India
Mishra N.	Indian Institute of Information Technology, Prayagraj, India
Mulpuru V.	Indian Institute of Information Technology, Prayagraj, India
Nagar P.K.	Indian Institute of Technology Kanpur, Kanpur, India
Nasibullah M.	Integral University, Lucknow, India
Patel D.K.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Rahman Q.I.	Integral University, Lucknow, India
Raza S.	Isabella Thoburn College, Lucknow, India
Sharma M.	Indian Institute of Technology Kanpur, Kanpur, India
Sharma P.	Babasaheb Bhim Rao Ambedkar University, Lucknow, India
Sharma V.P.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Singh N.	Amity University, Lucknow, India

Verma J. CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India

Yadav A. Indian Institute of Technology Kanpur, Kanpur, India

CHAPTER 10

Green Chemistry: Making Chemistry Environment-Friendly

Sangeeta Bajpai[1,*], **Saman Raza**[2], **Iqbal Azad**[3] and **Tahmeena Khan**[3]

[1] *Amity School of Applied Sciences, Amity University, Lucknow, India*

[2] *Isabella Thoburn College, Lucknow, India*

[3] *Integral University, Lucknow, India*

Abstract: Chemistry is all around the universe. Green chemistry underpins the enormous social and technological changes in the future. Beginning from eco-friendly chemical synthesis to green catalyst *via* green chemical reactions, it finds a good correlation with the environment, taking biosynthesis and biomimetic principles into consideration. Widespread interest in this field is seen today among scientists. Considering the present scenario of "The age of tools", the compatibility with technology today is of utmost importance. Green chemistry is one of the powerful tools to cut the Gordian knot of pollution by reducing chemicals in the surroundings to make them eco-friendly. This chapter emphasizes the various aspects of green chemistry, from its principles to its applications, leading to a sustainable eco-friendly future.

Keywords: Chemistry, Environment, Green chemistry, Pharmaceuticals, Solvent, Sustainable.

INTRODUCTION

Green Chemistry

Keeping an eye on the past and looking at the present, the fact that chemistry is often misused, cannot be denied. The increase in the percentage of pollutants, toxic substances, and non-biodegradable materials all around, has resulted in imbalanced biodiversity. Applications of chemistry on living systems to increase productivity without damaging our natural resources are a very important aspect today. Chemical industries are of utmost importance in the world's economy; however, their success has defaced the environment to some extent. Fortunately, scientists are moving steadily towards attaining an eco-friendly approach by

[*] **Corresponding author Sangeeta Bajpai:** Department of Chemistry, Amity School of Applied Sciences, Amity University, Lucknow, India; E-mail: sbajpai1@amity.edu

Tahmeena Khan, Abdul Rahman Khan, Saman Raza, Iqbal Azad and Alfred J. Lawrence (Eds.)