

Medicinal and Environmental Chemistry: Experimental Advances and Simulations

PART 1

Editors:

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



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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*

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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 xenoestrogens 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 1**Environmental Chemistry: Applications, Interactions and Paradigm Shift in Futuristic Approaches****Vinod Praveen Sharma^{1,*}, P. Sharma² and Abdul Rahman Khan³**¹ *CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India*² *Babasaheb Bhim Rao Ambedkar University, Lucknow, India*³ *Integral University, Lucknow, India*

Abstract: Environmental chemistry is an interdisciplinary science with multiple importance in the dynamic lifestyle and consumption pattern. Globally, the environmental regulatory agencies and research institutions feel the extreme need for environmental chemistry for the identification of the nature, source, monitoring, and remediation of pollutants. The pollutants may range from heavy metals, organometallics, polycyclic aromatic hydrocarbons, and nutrients, to the runoff of various other contaminants, their transportation, and interaction with living organisms. Their rapid and accurate separation, identification, quantification using sophisticated techniques, characterization, and understanding of the interactions and mechanisms are the key components of analytical chemistry, for better biochemical or physiological understanding. Contaminants generally have short or long-term toxic implications on the surrounding environment due to direct impact or through bioactivity. Management of environmental pollutants, with minimal impact on biodiversity and human population, is the desired objective of most of the Research & Development programs of International societal relevance. The coordination and effective implementation through sustainable, green, computational technologies may provide the best strategic solutions to the innovators, academicians, and stakeholders, amidst constraints on resources.

Keywords: Characterization, Environmental, Management, Strategic, Sustainable, Technologies.

INTRODUCTION

We need to attempt visualising the pathways and draw a roadmap for a sustainable future. We all know that newer materials/ alloys will lead to improved products, and novel processes may improve manufacturing efficiency and reduce

* **Corresponding author Vinod Praveen Sharma:** CSIR- Indian Institute of Toxicology Research, Mahatma Gandhi Marg, Lucknow, Uttar Pradesh; E-mail: vpsitr1@rediffmail.com