

Medicinal and Environmental Chemistry: Experimental Advances and Simulations

PART 2

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 II)

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

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Email: subscriptions@benthamscience.net



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FOREWORD

In recent years, our environment has deteriorated at an alarming rate. Be it the air we breathe, the water we drink, or the food we eat—the hazards are hitting closer to home. Consequently, there has been a deluge of diseases and disorders associated with environmental pollution, industrialization, lifestyle changes, etc. From cardiovascular diseases and growth defects to neurological disorders and stress, these environmental diseases have been coupled with other environmental threats like pollution, climate change, food shortage, and novel infections and have made the study of environmental chemistry indispensable in present times. In the development of more effective and safer therapies that would cater to diseases both old and new, the study of medicinal chemistry is vital to determine accurate knowledge of drugs, their structure, synthesis, pharmacology, and pharmacokinetics.

Environmental diseases have brought about a close association between these two branches of chemistry as well as pharmaceutical chemistry. It gives me great pleasure that this book brings them together on one platform. This book aims to provide a better comprehension of environmental problems as well as remedial strategies to amend them and includes an assorted collection of topics presented by experts from academia, research, and development.

I think that the authors can be confident that readers will gain a broader perspective of the disciplines of environmental chemistry, medicinal chemistry, and pharmaceutical chemistry as a result of their efforts.

Imran Ahmad
Jina Pharmaceuticals Inc.
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, including the novel corona virus 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 medicinal chemistry and environmental chemistry have been widely explored separately, 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.

The twenty-one chapters included in the book are focused on diverse topics trying to blend the fields of environmental chemistry and medicinal chemistry and have been authored by expert 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 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, antibiotics, and plastics, which have become a major source of pollution, along with their remediation. The biochemical aspect of Cytochrome P₄₅₀ and its association with mitigation strategy upon the exposure of smog on the human body, the effect of environmental xenoestrogens on human health, and the potential of natural curing agents to combat ecotoxicity have also been explored. Experimental techniques like the use of quantification methods for pharmaceuticals and persistent organic pollutants, chemosensors and polymeric ceramic composite membranes, and the concept of nanotechnology for the synthesis and use of gold and silver nanoparticles from plant-based sources have also been elaborated. To further elaborate on the importance of safe chemical practise, the concept of green chemistry has 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 to make futuristic and accurate predictions to make drug discovery efficient, quicker and cost-effective. Chapters summarizing the advances of biomolecular simulations for drug designing with respect to ecotoxicity, drug degradation, use of bioisosteric groups, and advances in pharmaceutical and modelling interventions for the treatment of COPD are also included. An interesting chapter has also explained the ligand identification for effective drug development through virtual screening by taking the example of COVID-19.

The book will prove beneficial for academicians, students of environmental chemistry and pharmacy, researchers, scientists, computational chemists, pharmacologists, environmentalists, policymakers, and postgraduate students. It would also provide researchers and medicinal chemists, information about 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

Agarwal S.	Isabella Thoburn College, Lucknow, India
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 A.	King George's Medical University, Lucknow, India Shibli National PG College, Azamgarh, India
Azad I.	Integral University, Lucknow, India
Azad M. I.	Jamia Millia Islamia, New Delhi, India
Bajpai S.	Amity University, Lucknow, India
Bhateria M.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Bhatia S.	Isabella Thoburn College, Lucknow, India
Bhateria M.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Bhatia S.	Isabella Thoburn College, Lucknow, India
Biswas K.	Indian Institute of Technology Kanpur, Kanpur, India
Dixit S.	CSIR-Central Institute of Medicinal and Aromatic Plants (CSIR-CIMAP), Lucknow, 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
Joshi S.	Isabella Thoburn College, Lucknow, India
Kant S.	King George's Medical University, Lucknow, India
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
Lawrence A. J.	Isabella Thoburn College, 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
Pandey J.	Amity 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
Rizvi A.	Previously at, CSIR- Central Drug Research Institute (CSIR-CDRI), 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
Shukla D.	S R Int, Knapur, India
Siddiq M.A.,	Jazan University, Jazan, Saudi Arabia
Singh N.	Amity University, Lucknow, India
Singh S. P.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Vankar P. S.	Bombay Textile Research Association, Mumbai, India
Verma J.	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Yadav A.	Indian Institute of Technology Kanpur, Kanpur, India

CHAPTER 3

Pharmaceutical and Modelling Interventions for Environmental Pollution Related Chronic Obstructive Pulmonary Disease

Tahmeena Khan¹, Alfred J. Lawrence², Iqal Azad¹, Shalini Dixit^{3,*} and Saman Raza²

¹ Integral University, Lucknow, India

² Isabella Thoburn College, Lucknow, India

³ CSIR-Central Institute of Medicinal and Aromatic Plants (CSIR-CIMAP), Lucknow, India

Abstract: Chronic obstructive lung diseases, including asthma and chronic obstructive pulmonary disease (COPD), are causing an extreme burden on societal health, affecting above 500 million people worldwide and affecting lung physiology at a multi-biological level. The increasing burden of air pollution is a major contributing factor to the disease, other than smoking and living conditions. Over the years, several studies have been undertaken to understand lung function, airflow mechanisms, and impairment for better therapies and therapeutic interventions. Still, it is very unlikely to predict the morbidity and mortality associated with COPD due to limitations of early and timely prediction and progression which calls for personalized treatment interventions to avert exacerbation and refractory symptoms. This chapter presents an overview of the status of COPD worldwide with a special emphasis on Indian statistics, along with the drug and pharmacological advancement, and computational medicinal modelling, its applications, and limitations. Though experimental models may predict the prerequisites for the system medicine approach, they are unable to analyse the finer details, calling for more advanced molecular technologies. A computational model of system medicine mimics the functioning of a complex system and can predict future functioning as well. Working with large data sets, computational models may have greater benefits to minimize patient risk and assist in clinical decision-making.

Keywords: Chemistry, COPD, Environment, Lung, Modelling, Pharmaceutical, Pollution.

* Corresponding author Shalini Dixit: Department of Analytical Chemistry, CSIR-Central Institute of Medicinal and Aromatic Plants, Lucknow, India; E-mail: shasddixit@gmail.com

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