

# 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

©2021, Bentham Books imprint.

Published by Bentham Science Publishers Pte. Ltd. Singapore. All Rights Reserved.

## **BENTHAM SCIENCE PUBLISHERS LTD.**

### **End User License Agreement (for non-institutional, personal use)**

This is an agreement between you and Bentham Science Publishers Ltd. Please read this License Agreement carefully before using the book/echapter/ejournal (“**Work**”). Your use of the Work constitutes your agreement to the terms and conditions set forth in this License Agreement. If you do not agree to these terms and conditions then you should not use the Work.

Bentham Science Publishers agrees to grant you a non-exclusive, non-transferable limited license to use the Work subject to and in accordance with the following terms and conditions. This License Agreement is for non-library, personal use only. For a library / institutional / multi user license in respect of the Work, please contact: [permission@benthamscience.net](mailto:permission@benthamscience.net).

### **Usage Rules:**

1. All rights reserved: The Work is the subject of copyright and Bentham Science Publishers either owns the Work (and the copyright in it) or is licensed to distribute the Work. You shall not copy, reproduce, modify, remove, delete, augment, add to, publish, transmit, sell, resell, create derivative works from, or in any way exploit the Work or make the Work available for others to do any of the same, in any form or by any means, in whole or in part, in each case without the prior written permission of Bentham Science Publishers, unless stated otherwise in this License Agreement.
2. You may download a copy of the Work on one occasion to one personal computer (including tablet, laptop, desktop, or other such devices). You may make one back-up copy of the Work to avoid losing it.
3. The unauthorised use or distribution of copyrighted or other proprietary content is illegal and could subject you to liability for substantial money damages. You will be liable for any damage resulting from your misuse of the Work or any violation of this License Agreement, including any infringement by you of copyrights or proprietary rights.

### ***Disclaimer:***

Bentham Science Publishers does not guarantee that the information in the Work is error-free, or warrant that it will meet your requirements or that access to the Work will be uninterrupted or error-free. The Work is provided "as is" without warranty of any kind, either express or implied or statutory, including, without limitation, implied warranties of merchantability and fitness for a particular purpose. The entire risk as to the results and performance of the Work is assumed by you. No responsibility is assumed by Bentham Science Publishers, its staff, editors and/or authors for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products instruction, advertisements or ideas contained in the Work.

### ***Limitation of Liability:***

In no event will Bentham Science Publishers, its staff, editors and/or authors, be liable for any damages, including, without limitation, special, incidental and/or consequential damages and/or damages for lost data and/or profits arising out of (whether directly or indirectly) the use or inability to use the Work. The entire liability of Bentham Science Publishers shall be limited to the amount actually paid by you for the Work.

### **General:**

1. Any dispute or claim arising out of or in connection with this License Agreement or the Work (including non-contractual disputes or claims) will be governed by and construed in accordance with the laws of Singapore. Each party agrees that the courts of the state of Singapore shall have exclusive jurisdiction to settle any dispute or claim arising out of or in connection with this License Agreement or the Work (including non-contractual disputes or claims).
2. Your rights under this License Agreement will automatically terminate without notice and without the

- 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](mailto:subscriptions@benthamscience.net)



## CONTENTS

FOREWORD .....	i
PREFACE .....	ii
LIST OF CONTRIBUTORS .....	iv
<b>CHAPTER 1 ENVIRONMENTAL CHEMISTRY: APPLICATIONS, INTERACTIONS AND PARADIGM SHIFT IN FUTURISTIC APPROACHES .....</b>	<b>1</b>
<i>Vinod Praveen Sharma, P. Sharma and Abdul Rahman Khan</i>	
INTRODUCTION .....	1
INDUSTRIALIZATION AND CHEMICAL RESEARCH WORKS .....	2
PARADIGM CHANGES AND INNOVATIONS .....	3
AGRICULTURAL CHEMISTRY AND GREENER HABITATIONS: INTERLINKS .....	4
FUTURISTIC APPROACHES .....	6
BIOMATERIALS .....	6
ENVIRONMENTAL CONSCIOUSNESS AND CARBON FOOTPRINT REDUCTION .....	7
NEW CHEMICAL ENTITIES AND STRUCTURE-ACTIVITY RELATIONSHIPS .....	7
INTERFACE BETWEEN MEDICINAL AND ENVIRONMENTAL CHEMISTRY .....	8
INFERENCES .....	11
CONCLUDING REMARKS .....	11
CONSENT FOR PUBLICATION .....	11
CONFLICT OF INTEREST .....	11
ACKNOWLEDGEMENT .....	12
REFERENCES .....	12
<b>CHAPTER 2 MEDICINAL CHEMISTRY: OPPORTUNITIES AND CHALLENGES .....</b>	<b>14</b>
<i>Jamal Akhtar Ansari, Abbas Ali Mahdi and Zafar Alam</i>	
INTRODUCTION .....	15
SOURCES OF A DRUG .....	15
SYNTHETIC SOURCES .....	16
PLANT-DERIVED SECONDARY METABOLITES/PHYTOCHEMICALS .....	20
MICROBIAL METABOLITES .....	23
MARINE INVERTEBRATES DERIVED COMPOUNDS .....	25
PORIFERA .....	26
CNIDARIA .....	26
MOLLUSCA .....	26
ARTHROPODA .....	27
RECOMBINANT DNA TECHNOLOGY .....	29
ANIMAL-BASED MEDICINES .....	29
DESIGNING OF NEW CHEMICAL ENTITIES (NCES) .....	30
DEGRADATION OF DRUGS .....	32
CHALLENGES IN MEDICINAL CHEMISTRY .....	34
CONCLUDING REMARKS .....	36
CONSENT FOR PUBLICATION .....	37
CONFLICT OF INTEREST .....	37
ACKNOWLEDGEMENT .....	37
REFERENCES .....	37
<b>CHAPTER 3 ENVIRONMENTAL XENOESTROGENS: DEVELOPMENTAL EFFECT ON CHANGING ENVIRONMENT, MOLECULAR MECHANISMS, AND HUMAN HEALTH .....</b>	<b>42</b>
<i>Atul Gupta and Imran Ahmad</i>	
INTRODUCTION .....	42

Estrogens .....	42
Biosynthesis of Estrogens .....	44
Glandular Estrogen Synthesis .....	44
Extra-glandular Synthesis .....	44
Classification of Estrogens .....	46
Steroidal Estrogens .....	46
Nonsteroidal Estrogens .....	48
Functions and Mechanism of Action of Estrogens .....	50
Estrogen Receptors .....	51
Xenoestrogens .....	53
Natural Environmental Estrogen .....	54
Synthetic Xenoestrogens .....	54
Mechanism of Action of Xenoestrogens .....	56
<i>a. Binding Directly to Estrogen Receptor</i> .....	56
<i>b. Other Plausible Mechanisms</i> .....	56
Sources of Xenoestrogens .....	57
Water .....	58
Chemical Pesticides and Fertilizers .....	58
Non-Organic Food Products .....	59
Plastics .....	59
Cosmetics and Toiletries .....	59
Phthalates .....	60
Parabens .....	60
Triclosan .....	60
Household Cleaners and Kitchen Ware .....	60
Pharmaceutical Products .....	61
Adverse Effects of Xenoestrogens .....	61
Xenoestrogens: Implications for Risk Assessment .....	62
Endocrine-Disrupting Chemicals affecting Reproduction .....	63
Suggestions .....	64
<b>CONCLUDING REMARKS</b> .....	65
<b>CONSENT FOR PUBLICATION</b> .....	66
<b>CONFLICT OF INTEREST</b> .....	66
<b>ACKNOWLEDGEMENT</b> .....	66
<b>REFERENCES</b> .....	66

<b>CHAPTER 4 PERSISTENT ORGANIC POLLUTANTS: THE ANCIENT INTRUDERS OF OUR ENVIRONMENT</b> .....	75
<i>Devendra Kumar Patel, Neha Gupta, Sandeep Kumar and Juhi Verma</i>	
<b>INTRODUCTION</b> .....	75
<b>ENVIRONMENTAL EFFECT OF POPS</b> .....	78
1. Pesticides .....	79
2. Dioxins, Furans, and Polychlorinated Biphenyls .....	80
3. Polybrominated Diphenyl Ethers (PBDEs) .....	80
4. Polycyclic Aromatic Hydrocarbons (PAHs) .....	81
<b>HEALTH EFFECT OF POPS</b> .....	81
Endocrine Disruptions .....	81
Reproductive Defects .....	82
Cardiovascular Problems .....	82
Cancer .....	82
Diabetes .....	83

<b>REMEDIATION</b> .....	85
Microbial Degradation .....	91
1. <i>Bacterial Degradation</i> .....	91
2. <i>Fungal Degradation</i> .....	91
3. <i>Algal Degradation</i> .....	92
<b>OXIDATION PROCESS FOR WASTEWATER TREATMENT</b> .....	92
<b>RECENT ADVANCEMENTS</b> .....	93
<b>CONCLUDING REMARKS</b> .....	93
<b>LIST OF ABBREVIATIONS</b> .....	94
<b>CONSENT FOR PUBLICATION</b> .....	94
<b>CONFLICT OF INTEREST</b> .....	94
<b>ACKNOWLEDGEMENT</b> .....	94
<b>REFERENCES</b> .....	94
<b>CHAPTER 5 AN EXPERIMENTAL AND SIMULATION STUDY TO ADDRESS VARIABILITIES AND UNCERTAINTIES IN RISK ASSESSMENT OF LEAD AND CADMIUM INGESTION FOR A VEGETARIAN DIET</b> .....	101
<i>Ashish Yadav, Kaniska Biswas, Mukesh Sharma, Arunima Khare and Pavan K.     Nagar</i>	
<b>INTRODUCTION</b> .....	102
<b>STUDY AREA, MATERIALS, AND METHOD</b> .....	103
<b>SAMPLE COLLECTION</b> .....	104
Food and Water Samples .....	104
<b>URINE SAMPLES</b> .....	105
<b>SAMPLE ANALYSIS</b> .....	106
Sample Processing .....	106
<b>INSTRUMENTATION AND ANALYSIS</b> .....	106
<b>URINE ANALYSIS</b> .....	107
<b>RISK ASSESSMENT METHODOLOGY</b> .....	107
<b>RESULTS AND DISCUSSION</b> .....	108
Concentration of Pb and Cd in Various Food Items .....	108
Risk Characterization .....	110
<i>Dietary Intake (Pb and Cd)</i> .....	110
<i>PbB-based Risk Assessment</i> .....	112
<i>CdU-based Risk Assessment</i> .....	113
<b>CONCLUDING REMARKS</b> .....	114
<b>CONSENT FOR PUBLICATION</b> .....	115
<b>CONFLICT OF INTEREST</b> .....	115
<b>ACKNOWLEDGEMENT</b> .....	115
<b>REFERENCES</b> .....	115
<b>CHAPTER 6 SAFETY EVALUATION OF COLOURED PLASTIC TIFFINS/BOTTLES AND MEDICAL STRATEGIES TO MITIGATE ADDITIVE TOXICITY</b> .....	119
<i>Sonika Bhatia</i>	
<b>INTRODUCTION</b> .....	119
<b>HEAVY METAL TOXICITY</b> .....	121
<b>TOXICITY MECHANISM</b> .....	121
<b>MEDICAL INTERVENTIONS AND STRATEGIES</b> .....	122
<b>COMMON CHELATING AGENTS IN USE</b> .....	123
<b>DIMERCAPROL</b> .....	123
<b>DMSA &amp; DMPS-ORAL CHELATION ANALOGUES OF DIMERCAPROL</b> .....	123
<b>SODIUM-CALCIUM EDTA</b> .....	123

<b>DEFEROXAMINE (DFO)</b> .....	123
<b>PENICILLAMINE AND TRIENTINE (TRITHYLENETETRAMINE)- ORAL COPPER CHELATORS</b> .....	124
<b>DMSA ANALOGUES</b> .....	124
<b>DEFERIPRONE AND DEFERASIROX-ORAL IRON CHELATORS</b> .....	125
<b>COMBINATION THERAPY</b> .....	125
<b>PHTHALATE TOXICITY</b> .....	125
<b>BISPHENOL A TOXICITY</b> .....	126
<b>THERAPEUTIC STRATEGIES TO REDUCE TOXICITY DUE TO PHTHALATES AND BPA</b> .....	127
<b>REDUCING EXPOSURE</b> .....	127
<b>INCREASING RATE OF ELIMINATION</b> .....	127
<b>ANTIOXIDANT SUPPLEMENTS</b> .....	127
<b>A CASE STUDY</b> .....	128
<b>RESULTS</b> .....	128
<b>HEAVY METAL MIGRATION (IN PPM)</b> .....	133
<b>SURVEY</b> .....	135
<b>OBJECTIVES</b> .....	135
<b>TOOLS USED</b> .....	136
<b>INTERPRETATION AND ANALYSIS OF SURVEY</b> .....	136
<b>AWARENESS BUILDING</b> .....	141
<b>CONCLUDING REMARKS</b> .....	141
<b>CONSENT FOR PUBLICATION</b> .....	142
<b>CONFLICT OF INTEREST</b> .....	142
<b>ACKNOWLEDGEMENT</b> .....	142
<b>REFERENCES</b> .....	142
<b>CHAPTER 7 NATURAL COMPOUNDS WITH ANTICANCER THERAPEUTIC POTENTIAL FOR COMBATING ECOTOXIC CARCINOGENS</b> .....	147
<i>Anamika Mishra and Nidhi Mishra</i>	
<b>INTRODUCTION</b> .....	147
<b>ENVIRONMENT: A RESERVOIR OF ECOTOXIC CARCINOGENS AND SOURCE OF ANTICANCER DRUGS</b> .....	149
Ecotoxic Carcinogens .....	149
Aflatoxins .....	149
Aristolochic Acids .....	150
Arsenic .....	151
Asbestos .....	152
Benzene .....	152
Beryllium .....	153
Cadmium .....	153
Chromium .....	153
Cigarette Smoke .....	154
Ionizing radiation .....	154
Environment for the Treatment of Cancer .....	155
Vinca Alkaloids .....	155
Taxanes .....	156
Podophyllotoxin .....	157
Camptothecin Derivatives .....	158
Colchicine .....	158
Combretastatin .....	159

<b>CONCLUDING REMARKS</b> .....	161
<b>CONSENT FOR PUBLICATION</b> .....	161
<b>CONFLICT OF INTEREST</b> .....	161
<b>ACKNOWLEDGEMENT</b> .....	161
<b>REFERENCES</b> .....	161
<b>CHAPTER 8 BASICS OF DRUG DESIGNING THROUGH SMALL ORGANIC MOLECULES AND THEIR TOXICOLOGICAL IMPACT ON THE ENVIRONMENT</b> .....	166
<i>Mohd Azhar Khan, Arif Ali, Fakhra Jabeen, Malik Nasibullah, Tahmeena Khan</i>	
<i>Musheer Ahmad and Qazi Inamur Rahman</i>	
<b>INTRODUCTION</b> .....	167
Drug Design and Development of New Drugs .....	167
The Procedure Followed in Drug Design .....	167
Concept of Lead Compounds and Lead Modifications .....	168
Concept of a Prodrug, Double Prodrug, and Soft Drug .....	168
<i>a. Prodrugs</i> .....	168
<i>i. Electronic nature</i> .....	169
<i>ii. Steric Factors</i> .....	169
<i>b. Double Prodrugs</i> .....	170
<i>c. Soft Drugs</i> .....	170
1. Soft Analogues .....	171
2. Activated Soft Compounds .....	172
3. Natural Soft Drug .....	172
4. Soft Drug Based on the Active Metabolite Approach .....	173
5. Soft Drug Based on the Inactive Metabolite Approach .....	173
Structure-Activity Relationship (SAR) .....	174
1. Effect of the Hydroxyl Group .....	174
2. Effect of Aldehydes and Ketones .....	175
3. Effect of Acidic Groups .....	175
4. Effect of Alkyl Groups .....	175
History and Development of QSAR (Quantitative Structure-activity Relationship) .....	177
Quantitative Structure-Activity Relationship (QSAR) methods .....	178
1. Free Wilson model .....	178
2. Hansch approach .....	178
Relationship Between free-Wilson and Hansch Analysis .....	179
Factors Affecting Bio-activity .....	179
<i>Spatial Considerations</i> .....	179
1. Optical Isomerism .....	179
<i>R, S System for Asymmetric Molecules</i> .....	179
<i>Optical Isomerism and Biological Activity</i> .....	180
2. Geometrical Isomerism .....	181
<i>Priority Order Based on Atomic Number</i> .....	181
<i>Geometrical Isomerism and Pharmacological Activity</i> .....	182
<i>Isosterism</i> .....	182
<i>Bio-isosterism</i> .....	183
<i>Redox Potentials</i> .....	184
<i>Theories of Drug Activity</i> .....	185
1. Receptor Theory .....	186
2. Occupancy Theory .....	186
3. Affinity and Intrinsic Activity .....	187
4. Charniere Theory .....	187

5. Rate Theory .....	187
6. Induced-fit-theory .....	188
<i>Concepts of Drug Receptors</i> .....	188
<i>Drug-Receptor Interaction</i> .....	188
<i>Physico-Chemical Parameters</i> .....	188
<i>Solubility Parameters or Lipophilic Parameters</i> .....	189
<i>Partition Coefficient Parameter</i> .....	189
<i>Surface Activity Parameters</i> .....	189
<i>Empirical Electronic Parameters</i> .....	190
<i>Ionization</i> .....	191
<i>Steric Parameters</i> .....	191
<i>Toxicological Effect of Drugs on the Environment</i> .....	191
<i>Effect of Drugs on the Environment</i> .....	192
<b>CONCLUDING REMARKS</b> .....	193
<b>CONSENT FOR PUBLICATION</b> .....	193
<b>CONFLICT OF INTEREST</b> .....	194
<b>ACKNOWLEDGEMENT</b> .....	194
<b>REFERENCES</b> .....	194
<b>CHAPTER 9 ADVANCES IN BIOMOLECULAR SIMULATIONS FOR RATIONAL DRUG DESIGNING AND ECOTOXICITY</b> .....	198
<i>Viswajit Mulpuru and Nidhi Mishra</i>	
<b>INTRODUCTION</b> .....	198
<b>VIRTUAL SCREENING</b> .....	199
<b>MOLECULAR DOCKING</b> .....	200
Rigid Docking .....	201
Semi-Flexible Docking .....	201
Flexible Docking .....	201
<b>ADMET ANALYSIS</b> .....	202
<b>MOLECULAR DYNAMICS</b> .....	202
General steps involved in Molecular Dynamics Simulation: .....	203
Energy Minimization .....	203
Solvation .....	204
Heating, Equilibration and Production Run .....	204
Analysis .....	205
Structural Visualization .....	205
Time Series and Thermodynamic Calculation .....	205
Quantitative Structure-Activity Relationship (QSAR) .....	206
Physiochemical Parameters .....	207
Hydrophobicity .....	207
The Partition Coefficient (P) .....	208
The Substituent Hydrophobicity Constant ( $\pi$ ) .....	208
Electronic Effects .....	208
Steric Factors .....	209
Hansch Equation .....	209
Pharmacokinetics and Pharmacodynamics .....	210
Absorption .....	211
Distribution .....	211
Metabolism .....	212
Excretion .....	212
Pharmacokinetic Models .....	212

The elimination rate constant .....	213
The volume of distribution .....	213
Half-Life .....	213
Clearance .....	214
Applications of Bioinformatic Techniques in Environmental Sciences .....	214
<b>CONCLUDING REMARKS .....</b>	<b>216</b>
<b>CONSENT FOR PUBLICATION .....</b>	<b>217</b>
<b>CONFLICT OF INTEREST .....</b>	<b>217</b>
<b>ACKNOWLEDGEMENT .....</b>	<b>218</b>
<b>REFERENCES .....</b>	<b>218</b>
<b>CHAPTER 10 GREEN CHEMISTRY: MAKING CHEMISTRY ENVIRONMENT-FRIENDLY</b> .....	<b>220</b>
<i>Sangeeta Bajpai, Saman Raza, Iqbal Azad and Tahmeena Khan</i>	
<b>INTRODUCTION .....</b>	<b>220</b>
Green Chemistry .....	220
Principles of Green Chemistry .....	221
Applications of Green Chemistry .....	226
1. Corrosion .....	226
2. Nanotechnology .....	227
3. Pharmaceuticals .....	228
Efficient and economic routes applied for Oligonucleotides Drugs .....	229
Analgesic and Anti-inflammatory Drugs .....	231
Use of Solvents .....	232
Solvent Pollution and Hazardous Environmental and Health Effects .....	233
Green Solvents as Environment-friendly Alternatives .....	234
Water .....	235
Glycerol .....	235
Supercritical Carbon Dioxide .....	236
Carbonic Esters .....	236
Vegetable Oils .....	236
Ionic Liquids .....	237
<b>CONCLUDING REMARKS .....</b>	<b>238</b>
<b>CONSENT FOR PUBLICATION .....</b>	<b>238</b>
<b>CONFLICT OF INTEREST .....</b>	<b>238</b>
<b>ACKNOWLEDGEMENT .....</b>	<b>238</b>
<b>REFERENCES .....</b>	<b>238</b>
<b>SUBJECT INDEX .....</b>	<b>244</b>

## **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

# Green Chemistry: Making Chemistry Environment-Friendly

Sangeeta Bajpai<sup>1,\*</sup>, Saman Raza<sup>2</sup>, Iqbal Azad<sup>3</sup> and Tahmeena Khan<sup>3</sup>

<sup>1</sup> Amity School of Applied Sciences, Amity University, Lucknow, India

<sup>2</sup> Isabella Thoburn College, Lucknow, India

<sup>3</sup> 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