

# Medicinal and Environmental Chemistry: Experimental Advances and Simulations

## PART 2

**Editors:**

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



**Bentham Books**

# **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*

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

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

ISBN (Online): 978-981-4998-30-7

ISBN (Print): 978-981-4998-31-4

ISBN (Paperback): 978-981-4998-32-1

©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 AIR POLLUTION AND ITS IMPACT ON RESPIRATORY HEALTH</b> .....	1
<i>Surya Kant</i>	
INTRODUCTION .....	1
MAJOR AIR POLLUTANTS .....	3
TYPES AND SOURCES OF AIR POLLUTION .....	3
Primary Air Pollutants .....	3
Secondary Air Pollutants .....	4
AIR POLLUTION CAN BE OF TWO TYPES .....	4
SECOND-HAND SMOKE .....	4
PARTICULATE MATTER (PM) .....	5
NATIONAL AIR QUALITY INDEX .....	6
OZONE (O <sub>3</sub> ) .....	7
CARBON MONOXIDE (CO) .....	8
NITROGEN OXIDES (NOX) .....	8
SULFUR DIOXIDE (SO <sub>2</sub> ) .....	8
LEAD .....	8
IMPACT OF AIR POLLUTION ON HEALTH .....	9
PREVENTION OF AIR POLLUTION .....	12
STRATEGIES AND SOLUTION .....	13
PRADHAN MANTRI UJJWALA YOJANA .....	13
PLANTATION .....	13
CONCLUDING REMARKS .....	14
Suggestions of the Author to Combat Air Pollution .....	14
CONSENT FOR PUBLICATION .....	14
CONFLICT OF INTEREST .....	14
ACKNOWLEDGEMENT .....	14
REFERENCES .....	14
<b>CHAPTER 2 CYTOCHROME P450 AND HEALTH HAZARDS OF SMOG</b> .....	18
<i>Amber Rizvi</i>	
INTRODUCTION .....	18
TYPES OF SMOG .....	19
HEALTH HAZARDS OF SMOG .....	20
CYTOCHROME P450 .....	20
DISEASES CAUSED BY SMOG AND ITS EFFECT ON CYPs .....	22
Myocardial Infarction (MI) .....	22
Mechanism of Cardiotoxicity of Air Pollutants .....	23
Role of CYPs in MIs .....	23
Chronic Obstructive Pulmonary Disease (COPD) .....	24
CYPs and COPD .....	25
Atopic Dermatitis (Eczema) .....	26
CYPs and Atopic Dermatitis .....	27
Coughing .....	27
CYPs and Coughing .....	28
Experimental Work Done on CYP .....	28

CONCLUDING REMARKS .....	29
CONSENT FOR PUBLICATION .....	30
CONFLICT OF INTEREST .....	30
ACKNOWLEDGEMENT .....	30
REFERENCES .....	30
<b>CHAPTER 3 PHARMACEUTICAL AND MODELLING INTERVENTIONS FOR ENVIRONMENTAL POLLUTION RELATED CHRONIC OBSTRUCTIVE PULMONARY DISEASE .....</b>	<b>32</b>
<i>Tahmeena Khan, Alfred J. Lawrence, Iqal Azad, Shalini Dixit and Saman Raza</i> .....	
<b>INTRODUCTION .....</b>	<b>33</b>
<b>INFLUENCING FACTORS FOR INITIATION AND MODULATION .....</b>	<b>33</b>
<b>COPD AND ITS ASSOCIATION WITH COMMON AIR POLLUTANTS: A WORLDWIDE PERSPECTIVE .....</b>	<b>34</b>
<b>COPD AND ITS STATUS IN INDIA .....</b>	<b>35</b>
<b>MECHANISTIC ACTION OF COPD- THE CHEMICAL AND BIOCHEMICAL APPROACH .....</b>	<b>36</b>
<b>OXIDATIVE STRESS .....</b>	<b>36</b>
<b>PROTEASE-ANTIPROTEASE IMBALANCE .....</b>	<b>37</b>
<b>ROLE OF MEDIATORS .....</b>	<b>37</b>
<b>DRUG AND PHARMACOLOGICAL ADVANCEMENT .....</b>	<b>38</b>
Tissue and Systematic Inflammation .....	38
<b>PHARMACEUTICAL INTERVENTIONS .....</b>	<b>38</b>
Corticosteroids .....	38
Bronchodilators .....	39
SABA (Short-acting Inhaled Beta-agonists) .....	39
SABA & SAMA (Short-acting Muscarinic Antagonist) Combination Bronchodilators .....	39
Long-Acting Bronchodilators .....	39
Combination Therapies .....	40
Combination of Corticosteroids and Long-acting Bronchodilators .....	40
Triple Therapy .....	41
Combination of Inhaled Corticosteroids and Two Long-acting Bronchodilators (Triple Therapy) .....	41
Other Options .....	41
Drawbacks and Need for System Medicinal Approach .....	41
Simulated Medicinal Modeling and its Significance .....	42
<b>COMPUTATIONAL MEDICINAL SIMULATION FOR COPD TREATMENT .....</b>	<b>43</b>
Computational Lung Modelling .....	43
Multiscale Modelling .....	44
Mechanistic Models .....	45
Machine Learning Models .....	45
Statistical models .....	46
COPD and Advancement in Modelling .....	46
COPD Progression Modelling .....	46
Experimental vs. Computational medicinal modelling .....	47
<b>LIMITATIONS AND NEED FOR FUTURE ADVANCEMENT .....</b>	<b>48</b>
<b>CONCLUDING REMARKS .....</b>	<b>49</b>
<b>CONSENT FOR PUBLICATION .....</b>	<b>50</b>
<b>CONFLICT OF INTEREST .....</b>	<b>50</b>
<b>ACKNOWLEDGEMENT .....</b>	<b>50</b>
<b>REFERENCES .....</b>	<b>50</b>

<b>CHAPTER 4 ARSENIC TOXICITY OF GROUNDWATER AND ITS REMEDIATION FOR DRINKING WATER</b> .....	58
<i>Seema Joshi</i>	
<b>INTRODUCTION</b> .....	58
<b>ESSENTIAL METALS</b> .....	59
<b>NON-ESSENTIAL METALS</b> .....	59
<b>CONCEPT OF TOXICITY</b> .....	59
1. Solubility of the Metal Complexes .....	60
2. Oxidation State of the Metal .....	60
3. Ligand Attached to the Metal Atom .....	60
<b>DETECTION OF METALS</b> .....	61
<b>TREATMENT FOR POISONING</b> .....	61
<b>ROLE OF METALS IN BIOLOGY</b> .....	61
<b>SOURCES OF ARSENIC</b> .....	63
<b>POTENTIAL FOR HUMAN EXPOSURE WITH SPECIAL EMPHASIS TO UTTAR PRADESH, INDIA</b> .....	63
Districts at High Risk .....	64
District at Moderate Risk .....	64
<b>MECHANISMS OF TOXICITY</b> .....	65
<b>CONSEQUENCES OF TOXICITY</b> .....	65
<b>REMEDICATION OF ARSENIC TOXICITY</b> .....	66
<b>CHELATING DRUGS USED IN THE TREATMENT OF ARSENIC POISONING</b> .....	68
1. Dimercaprol (BAL) .....	68
2. Dimercaptosuccinic Acid (DMSA) .....	69
3. 2,3-Dimercapto-1-propanesulfonic Acid (DMPS) .....	69
4. Penicillamine .....	70
<b>CHALLENGES OF CHELATION THERAPY</b> .....	70
<b>CASE STUDY FOR THE REMOVAL OF ARSENIC</b> .....	71
<b>CHEMICALS AND REAGENTS</b> .....	71
<b>PREPARATION OF FERRIC HYDROXIDE</b> .....	71
<b>REMOVAL OF ARSENIC FROM SPIKED TAP WATER USING FERRIC HYDROXIDE</b> .....	72
<b>PREPARATION OF IRON COATED CHARCOAL/SAND</b> .....	72
<b>EXPERIMENTAL DESIGN</b> .....	72
<b>CHARCOAL TREATMENT</b> .....	72
Iron Coated Charcoal Treatment .....	73
Iron Coated Coarse Sand Treatment .....	73
<b>DETERMINATION OF ARSENIC</b> .....	73
<b>FINDINGS OF THE STUDY</b> .....	73
<b>CONCLUDING REMARKS</b> .....	76
<b>CONSENT FOR PUBLICATION</b> .....	76
<b>CONFLICT OF INTEREST</b> .....	76
<b>ACKNOWLEDGEMENT</b> .....	76
<b>REFERENCES</b> .....	76
<b>CHAPTER 5 STUDIES ON POLYMERIC CERAMIC COMPOSITE MEMBRANES FOR WATER TREATMENT</b> .....	82
<i>Fakhra Jabeen, Qazi Inamur Rahman and Miad Ali Siddiq</i>	
<b>INTRODUCTION</b> .....	82
<b>WATER POLLUTION</b> .....	84
<b>PARAMETERS OF POLLUTION</b> .....	85
<b>MAIN SOURCES OF POLLUTANTS</b> .....	86

<b>MEMBRANES AND THEIR CLASSIFICATION</b> .....	88
Synthetic Membrane .....	88
Biological Membrane .....	89
Organic Membranes .....	89
Inorganic Membrane .....	89
Metallic Membranes .....	90
Ceramic Membranes .....	90
Micro-Porous Membranes .....	90
Meso-Porous Membranes .....	91
Macro Porous Membranes .....	91
<b>APPLICATIONS OF CERAMIC MEMBRANES</b> .....	97
Chemical Industry .....	97
Metal Industry/Surface Engineering .....	97
Textiles/Pulp and Paper Industry .....	98
Food and Beverages .....	98
Recycling and the Environment .....	98
<b>POLYETHERSULFONE MEMBRANE CHARACTERISTICS AND ITS TYPES</b> .....	100
<b>DESALINATION FOR WATER TREATMENT</b> .....	102
<b>TYPES OF DESALINATION PROCESSES</b> .....	104
<b>ADVANTAGES AND DISADVANTAGES OF DIFFERENT DESALINATION PROCESSES</b> .....	105
<b>CONCLUDING REMARKS</b> .....	110
<b>CONSENT FOR PUBLICATION</b> .....	111
<b>CONFLICT OF INTEREST</b> .....	111
<b>ACKNOWLEDGEMENT</b> .....	111
<b>REFERENCES</b> .....	111
<b>CHAPTER 6 CHEMOSENSORS FOR ANIONS OF BIOLOGICAL AND ENVIRONMENTAL RELEVANCE</b> .....	115
<i>Shweta Agarwal</i>	
<b>INTRODUCTION</b> .....	115
Biological Significance of Anions .....	116
Important Techniques for Detection of Anions .....	118
Ion Chromatography (IC) .....	118
Capillary Electrophoresis (CE) .....	118
Chemosensors .....	119
Optical Chemosensors for Anions .....	120
<i>Challenges in Development of Chemosensors</i> .....	120
Sensing Mechanisms of Chemosensors .....	122
Binding Site-Signalling Subunit Approach .....	122
Displacement Approach .....	123
Chemodosimeter Approach .....	123
Optical (Colourimetric and Fluorescence) Chemosensors for Anions .....	123
Optical Anion Sensing by Discrete molecules .....	124
Hydrogen Bond Chemosensors .....	124
Halogen Bond Chemosensors .....	126
Boron Based Lewis Acid Chemosensors .....	127
Metal Complexes as Chemosensors .....	128
Anion- $\pi$ Chemosensors .....	130
Chemosensors Based on Electrostatic Interactions .....	131
Chemodosimeters .....	131

Optical Sensing by Molecular Assemblies .....	133
<b>CONCLUDING REMARKS</b> .....	134
<b>LIST OF ABBREVIATIONS</b> .....	134
<b>CONSENT FOR PUBLICATION</b> .....	135
<b>CONFLICT OF INTEREST</b> .....	135
<b>ACKNOWLEDGEMENT</b> .....	135
<b>REFERENCES</b> .....	135
<b>CHAPTER 7 ANTIBIOTIC POLLUTION: CHALLENGES AND STRATEGIES</b> .....	141
<i>Saman Raza and Tahmeena Khan</i>	
<b>INTRODUCTION</b> .....	141
<b>MECHANISM OF ACTION OF ANTIBIOTICS</b> .....	144
i. Inhibition of Bacterial Cell Wall Synthesis .....	144
ii. Inhibition of Bacterial Protein Synthesis .....	145
iii. Disruption of Cell Membranes .....	145
iv. Inhibition of Nucleic Acid Synthesis .....	145
v. Antimetabolite Activity .....	145
<b>USES OF ANTIBIOTICS</b> .....	146
<b>ANIMAL FARMING</b> .....	146
<b>AGRICULTURAL PURPOSES</b> .....	146
<b>AQUACULTURE</b> .....	146
<b>ANTIBIOTIC POLLUTION</b> .....	147
<b>EFFECTS OF ANTIBIOTIC POLLUTION</b> .....	148
<b>EFFECT OF ANTIBIOTIC POLLUTION ON HEALTH: ANTIBIOTIC RESISTANCE</b> ...	149
<b>EFFECTS OF ANTIBIOTIC POLLUTION ON THE ENVIRONMENT</b> .....	150
<b>STRATEGIES TO COUNTER ANTIBIOTIC POLLUTION AND RESISTANCE</b> .....	151
A. Methods for the Reduction of Antibiotic Pollution .....	151
1. <i>Removal of Antibiotic Residues from Water</i> .....	151
2. <i>Reduction in the Use of Antibiotics</i> .....	152
B. Methods to Counter Antibiotic Resistance .....	154
1. <i>Adjuvant Therapy</i> .....	154
2. <i>Development of New Antibiotics</i> .....	158
<b>CONCLUDING REMARKS</b> .....	160
<b>CONSENT FOR PUBLICATION</b> .....	160
<b>CONFLICT OF INTEREST</b> .....	160
<b>ACKNOWLEDGEMENT</b> .....	161
<b>REFERENCES</b> .....	161
<b>CHAPTER 8 ANALYTICAL ADVANCEMENT FOR PHARMACEUTICALS</b>	
<b>QUANTIFICATION IN ENVIRONMENTAL MATRICES</b> .....	166
<i>Anushka Pandey, Manisha Bhatia and Sheelendra Pratap Singh</i>	
<b>INTRODUCTION</b> .....	167
Analytical Methods for the Determination of Pharmaceutical Residues in the Environment	168
Sample Preservation .....	169
i. <i>Filtration</i> .....	169
ii. <i>Non-acidic Preservative Agent</i> .....	169
iii. <i>Acidifying Agents</i> .....	170
Sample Preparation .....	171
i. <i>Liquid-Liquid Extraction (LLE)</i> .....	171
ii. <i>Dispersive Liquid-liquid Microextraction (DLLME)</i> .....	174
iii. <i>Solid – Phase Extraction (SPE)</i> .....	176
iv. <i>Solid-Phase Micro Extraction (SPME)</i> .....	179

v. <i>Stir- bar Sorptive Extraction (SBSE)</i> .....	181
Chromatographic Techniques for Pharmaceuticals Analysis .....	183
Analysis of Pharmaceutical Compounds by Gas Chromatography (GC) .....	183
Analysis of Pharmaceutical Compounds by Liquid Chromatography (LC) .....	186
Methods Used for the Analysis of Pharmaceuticals in Different Environmental Analysis ....	187
<b>CONCLUDING REMARKS</b> .....	193
<b>CONSENT FOR PUBLICATION</b> .....	193
<b>CONFLICT OF INTEREST</b> .....	193
<b>ACKNOWLEDGEMENT</b> .....	193
<b>REFERENCES</b> .....	193
<b>CHAPTER 9 USE OF BIOISOSTERIC FUNCTIONAL GROUP REPLACEMENTS OR MODIFICATIONS FOR IMPROVED ENVIRONMENTAL HEALTH</b> .....	198
<i>Nidhi Singh and Jaya Pandey</i>	
<b>INTRODUCTION</b> .....	198
<b>BIOISOSTERISM - DIRECT EFFECT ON ENVIRONMENT</b> .....	199
<b>BIOISOSTERIC MODIFICATIONS FOR ANTHRANILIC DIAMIDES</b> .....	200
<b>BIOISOSTERIC MODIFICATIONS AT AROMATIC BRIDGED AMIDE FUNCTIONAL GROUP</b> .....	200
<b>BIOISOSTERIC MODIFICATIONS AT ALIPHATIC AMIDE FUNCTIONAL GROUPS</b> .....	203
<b>BIOISOSTERIC MODIFICATIONS FOR ORGANOCHLORINES</b> .....	205
<b>BIOISOSTERISM - INDIRECT EFFECT ON ENVIRONMENT</b> .....	206
<b>BIOISOSTERIC MODIFICATIONS FOR DIARYLPYRIMIDINE DERIVATIVES</b> .....	207
<b>BIOISOSTERIC MODIFICATIONS FOR CARBOHYDRATES</b> .....	208
<b>SOME IMPORTANT EXAMPLES OF BIOISOSTERIC FUNCTIONAL GROUP MODIFICATIONS FOR IMPROVED ENVIRONMENT</b> .....	211
1. Ivacaftor .....	211
2. Tetrabenazine .....	211
3. JNJ-38877605 .....	212
4. SCH-48461 .....	212
5. Etofenprox .....	213
6. Trifluoromethyl Ketone .....	213
7. Pulegone .....	214
8. Efavirenz .....	215
9. Iloprost .....	215
10. L-158809 .....	216
<b>CONCLUDING REMARKS</b> .....	216
<b>CONSENT FOR PUBLICATION</b> .....	217
<b>CONFLICT OF INTEREST</b> .....	217
<b>ACKNOWLEDGEMENT</b> .....	217
<b>REFERENCES</b> .....	217
<b>CHAPTER 10 GOLD AND SILVER NANOPARTICLE SYNTHESIS BY PYRUS AND EURYA: ENVIRONMENT-FRIENDLY THERAPEUTIC AGENTS</b> .....	220
<i>Dhara Shukla and Padma S. Vankar</i>	
<b>INTRODUCTION</b> .....	221
<b>MATERIAL AND METHODS</b> .....	223
Material Collection .....	223
Instrumentation .....	223
Preparation of Bio-Extract .....	224
<b>RESULTS AND DISCUSSION</b> .....	224

Morphological Identification of Gold and Silver Nanoparticles Produced by Eurya acuminata Leaves .....	226
Effect of the Presence of Metal Ions on Nanoparticle formation .....	228
Biomedical or Therapeutic Applications Involving Gold and Silver NPs .....	229
<b>CONCLUDING REMARKS</b> .....	231
<b>LIST OF ABBREVIATIONS</b> .....	232
<b>CONSENT FOR PUBLICATION</b> .....	233
<b>CONFLICT OF INTEREST</b> .....	233
<b>ACKNOWLEDGEMENT</b> .....	233
<b>REFERENCES</b> .....	233
<b>CHAPTER 11 NOVEL DRUG DEVELOPMENT STRATEGIES- A CASE STUDY WITH SARS-COV-2</b> .....	238
<i>Iqbal Azad, Tahmeena Khan, Mohammad Irfan Azad and Abdul Rahman Khan</i>	
<b>INTRODUCTION</b> .....	238
<b>FACTORS AFFECTING THE SPREAD OF SARS-COV-2</b> .....	239
Environmental Factors .....	239
Food Materials, Handlers, and Packaging .....	240
Water and Wastewater .....	240
Air .....	241
Insects .....	241
Medicinal Intervention: The Scope of Virtual Screening .....	242
<i>Structure-based Virtual Screening (SBVS)</i> .....	242
<i>Ligand-based Virtual Screening (LBVS)</i> .....	242
In-silico Approaches .....	243
<b>LIGAND SELECTION CRITERION AS PHARMACEUTICAL LEADS</b> .....	243
<b>LIPINSKI'S RULE OF FIVE</b> .....	243
<b>GHOSE FILTER</b> .....	244
<b>VEBER'S RULES</b> .....	244
<b>MDDR-LIKE RULES</b> .....	244
<b>CMC LIKE RULES</b> .....	245
<b>WDI-LIKE RULES</b> .....	245
<b>BAYER FILTER</b> .....	245
<b>RULE OF THREE</b> .....	245
<b>WEIGHTED AND UNWEIGHTED QED</b> .....	245
<b>DRUG REPURPOSING</b> .....	246
<b>DRUG REPURPOSING ADVANTAGES</b> .....	246
<b>DRUG CANDIDATE SELECTION</b> .....	247
<b>DETECTION OF TARGETS FOR DRUGS AND THEIR MECHANISM OF ACTION</b> .....	247
<b>MOLECULAR DOCKING</b> .....	247
<b>TYPES OF MOLECULAR DOCKING</b> .....	248
<b>FLEXIBLE DOCKING</b> .....	248
<b>FLEXIBLE DOCKING: CHALLENGES AND REQUIREMENTS</b> .....	248
<b>RIGID DOCKING: CHALLENGES AND REQUIREMENTS</b> .....	249
<b>MOLECULAR DOCKING STUDIES OF PLANT-BASED ACTIVE CONSTITUENTS IN SEARCH OF A LEAD MOLECULE TO COMBAT SARS-COV-2</b> .....	249
Role of Immunity .....	249
<b>PLANT-BASED RESOURCES AS NATURAL IMMUNITY BOOSTERS</b> .....	250
<b>GINGER (ZINGIBER OFFICINALE)</b> .....	250
<b>GARLIC (ALLIUM SATIVUM L.)</b> .....	252
<b>GREEN TEA (CAMELLIA SINENSIS)</b> .....	252

<b>PURPLE CONEFLOWER (ECHINACEA)</b> .....	253
<b>BLACK CUMIN (NIGELLA SATIVA)</b> .....	253
<b>CITRUS FRUITS</b> .....	253
<b>MOLECULAR DOCKING STUDIES WITH SOME BIOACTIVE CONSTITUENTS OF</b>	
<b>CITRUS FRUITS</b> .....	254
<b>SOFTWARES USED</b> .....	254
<b>THE OPEN READING FRAME (ORF)</b> .....	255
<b>TARGET PROTEINS</b> .....	255
Polyproteins (Proteases) .....	255
<b>SPIKE (S) PROTEIN</b> .....	255
<b>NUCLEOCAPSID (N) PROTEIN</b> .....	255
<b>ENVELOPE (E) PROTEIN</b> .....	256
<b>M-PROTEIN</b> .....	256
<b>SARS-COV HELICASE</b> .....	256
<b>PREPARATION OF THE RECEPTOR FOR DOCKING</b> .....	257
<b>PREPARATION OF LIGANDS FOR DOCKING</b> .....	257
<b>AUTODOCK VINA</b> .....	258
<b>IGEMDOCK</b> .....	258
<b>RESULTS AND DISCUSSION</b> .....	259
<b>CONCLUDING REMARKS</b> .....	261
<b>CONSENT FOR PUBLICATION</b> .....	261
<b>CONFLICT OF INTEREST</b> .....	261
<b>ACKNOWLEDGEMENT</b> .....	261
<b>REFERENCES</b> .....	261
<b>SUBJECT INDEX</b> .....	268

## 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 P<sub>450</sub> 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