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

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CONTENTS

FOREWORD i

PREFACE ii

LIST OF CONTRIBUTORS iv

CHAPTER 1 ENVIRONMENTAL CHEMISTRY: APPLICATIONS, INTERACTIONS AND PARADIGM SHIFT IN FUTURISTIC APPROACHES 1

Vinod Praveen Sharma, P. Sharma and *Abdul Rahman Khan*

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

CHAPTER 2 MEDICINAL CHEMISTRY: OPPORTUNITIES AND CHALLENGES 14

Jamal Akhtar Ansari, Abbas Ali Mahdi and *Zafar Alam*

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

CHAPTER 3 ENVIRONMENTAL XENOESTROGENS: DEVELOPMENTAL EFFECT ON CHANGING ENVIRONMENT, MOLECULAR MECHANISMS, AND HUMAN HEALTH 42

Atul Gupta and *Imran Ahmad*

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
a. Binding Directly to Estrogen Receptor 56
b. Other Plausible Mechanisms 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
CONCLUDING REMARKS 65
CONSENT FOR PUBLICATION 66
CONFLICT OF INTEREST 66
ACKNOWLEDGEMENT 66
REFERENCES 66

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

REMEDIATION 85
Microbial Degradation 91
1. Bacterial Degradation 91
2. Fungal Degradation 91
3. Algal Degradation 92
OXIDATION PROCESS FOR WASTEWATER TREATMENT 92
RECENT ADVANCEMENTS 93
CONCLUDING REMARKS 93
LIST OF ABBREVIATIONS 94
CONSENT FOR PUBLICATION 94
CONFLICT OF INTEREST 94
ACKNOWLEDGEMENT 94
REFERENCES 94

CHAPTER 5 AN EXPERIMENTAL AND SIMULATION STUDY TO ADDRESS VARIABILITIES AND UNCERTAINTIES IN RISK ASSESSMENT OF LEAD AND CADMIUM INGESTION FOR A VEGETARIAN DIET 101
Ashish Yadav, Kaniska Biswas, Mukesh Sharma, Arunima Khare and *Pavan K. Nagar*
INTRODUCTION 102
STUDY AREA, MATERIALS, AND METHOD 103
SAMPLE COLLECTION 104
Food and Water Samples 104
URINE SAMPLES 105
SAMPLE ANALYSIS 106
Sample Processing 106
INSTRUMENTATION AND ANALYSIS 106
URINE ANALYSIS 107
RISK ASSESSMENT METHODOLOGY 107
RESULTS AND DISCUSSION 108
Concentration of Pb and Cd in Various Food Items 108
Risk Characterization 110
Dietary Intake (Pb and Cd) 110
PbB-based Risk Assessment 112
CdU-based Risk Assessment 113
CONCLUDING REMARKS 114
CONSENT FOR PUBLICATION 115
CONFLICT OF INTEREST 115
ACKNOWLEDGEMENT 115
REFERENCES 115

CHAPTER 6 SAFETY EVALUATION OF COLOURED PLASTIC TIFFINS/BOTTLES AND MEDICAL STRATEGIES TO MITIGATE ADDITIVE TOXICITY 119
Sonika Bhatia
INTRODUCTION 119
HEAVY METAL TOXICITY 121
TOXICITY MECHANISM 121
MEDICAL INTERVENTIONS AND STRATEGIES 122
COMMON CHELATING AGENTS IN USE 123
DIMERCAPROL 123
DMSA & DMPS-ORAL CHELATION ANALOGUES OF DIMERCAPROL 123
SODIUM-CALCIUM EDTA 123

DEFEROXAMINE (DFO) 123
PENICILLAMINE AND TRIENTINE (TRITHYLENETETRAMINE)– ORAL COPPER CHELATORS 124
DMSA ANALOGUES 124
DEFERIPRONE AND DEFERASIROX-ORAL IRON CHELATORS 125
COMBINATION THERAPY 125
PHTHALATE TOXICITY 125
BISPHENOL A TOXICITY 126
THERAPEUTIC STRATEGIES TO REDUCE TOXICITY DUE TO PHTHALATES AND BPA 127
REDUCING EXPOSURE 127
INCREASING RATE OF ELIMINATION 127
ANTIOXIDANT SUPPLEMENTS 127
A CASE STUDY 128
RESULTS 128
HEAVY METAL MIGRATION (IN PPM) 133
SURVEY 135
OBJECTIVES 135
TOOLS USED 136
INTERPRETATION AND ANALYSIS OF SURVEY 136
AWARENESS BUILDING 141
CONCLUDING REMARKS 141
CONSENT FOR PUBLICATION 142
CONFLICT OF INTEREST 142
ACKNOWLEDGEMENT 142
REFERENCES 142

CHAPTER 7 NATURAL COMPOUNDS WITH ANTICANCER THERAPEUTIC POTENTIAL FOR COMBATING ECOTOXIC CARCINOGENS 147
Anamika Mishra and *Nidhi Mishra*
INTRODUCTION 147
ENVIRONMENT: A RESERVOIR OF ECOTOXIC CARCINOGENS AND SOURCE OF ANTICANCER DRUGS 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

CONCLUDING REMARKS 161
CONSENT FOR PUBLICATION 161
CONFLICT OF INTEREST 161
ACKNOWLEDGEMENT 161
REFERENCES 161

CHAPTER 8 BASICS OF DRUG DESIGNING THROUGH SMALL ORGANIC MOLECULES AND THEIR TOXICOLOGICAL IMPACT ON THE ENVIRONMENT 166
Mohd Azhar Khan, Arif Ali, Fakhra Jabeen, Malik Nasibullah, Tahmeena Khan Musheer Ahmad and *Qazi Inamur Rahman*
INTRODUCTION 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
a. Prodrugs 168
i. Electronic nature 169
ii. Steric Factors 169
b. Double Prodrugs 170
c. Soft Drugs 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
Spatial Considerations 179
1. Optical Isomerism 179
R, S System for Asymmetric Molecules 179
Optical Isomerism and Biological Activity 180
2. Geometrical Isomerism 181
Priority Order Based on Atomic Number 181
Geometrical Isomerism and Pharmacological Activity 182
Isosterism 182
Bio-isosterism 183
Redox Potentials 184
Theories of Drug Activity 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
Concepts of Drug Receptors 188
Drug-Receptor Interaction 188
Physico-Chemical Parameters 188
Solubility Parameters or Lipophilic Parameters 189
Partition Coefficient Parameter 189
Surface Activity Parameters 189
Empirical Electronic Parameters 190
Ionization 191
Steric Parameters 191
Toxicological Effect of Drugs on the Environment 191
Effect of Drugs on the Environment 192
CONCLUDING REMARKS 193
CONSENT FOR PUBLICATION 193
CONFLICT OF INTEREST 194
ACKNOWLEDGEMENT 194
REFERENCES 194

CHAPTER 9 ADVANCES IN BIOMOLECULAR SIMULATIONS FOR RATIONAL DRUG DESIGNING AND ECOTOXICITY 198
Viswajit Mulpuru and *Nidhi Mishra*
INTRODUCTION 198
VIRTUAL SCREENING 199
MOLECULAR DOCKING 200
Rigid Docking 201
Semi-Flexible Docking 201
Flexible Docking 201
ADMET ANALYSIS 202
MOLECULAR DYNAMICS 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 (π) 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
CONCLUDING REMARKS 216
CONSENT FOR PUBLICATION 217
CONFLICT OF INTEREST 217
ACKNOWLEDGEMENT 218
REFERENCES 218

CHAPTER 10 GREEN CHEMISTRY: MAKING CHEMISTRY ENVIRONMENT-FRIENDLY 220
Sangeeta Bajpai, Saman Raza, Iqbal Azad and *Tahmeena Khan*
INTRODUCTION 220
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
CONCLUDING REMARKS 238
CONSENT FOR PUBLICATION 238
CONFLICT OF INTEREST 238
ACKNOWLEDGEMENT 238
REFERENCES 238

SUBJECT INDEX 244

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 8

Basics of Drug Designing Through Small Organic Molecules and Their Toxicological Impact on The Environment

Mohd Azhar Khan[1], Arif Ali[2], Fakhra Jabeen[3], Malik Nasibullah[4], Tahmeena Khan[4], Musheer Ahmad[2,*] and **Qazi Inamur Rahman[4]**

[1] *K.K.L.Mahavidyala, Kanpur, India*

[2] *Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, India*

[3] *Samtah Jazan University, Kingdom of Saudi Arabia.*

[4] *Integral University, Lucknow, India*

Abstract: In the most basic sense, drug design involves designing molecules that are complementary in shape and charge to the biomolecular target with which they interact, and therefore will bind to it. The therapeutic potential of an organic molecule-based chemotherapeutic candidate is influenced by the basic functional groups, where the stereo-arrangement and stereo-selectivity of groups enhance the therapeutic benefits. Stereo-selective organic molecules in different configurations show diverse activity, such as (R) and (S) enantiomers of ibuprofen are effective pain killers but only (S) naproxen has inflammatory activity. Similarly, the transformation of diethyl stilbesterol has potential estrogenic activity and not the cis form. The softness or hardness of drugs depends on the functionality of organic molecules; mostly, the presence of hydroxyl and carboxylic groups improves the softness. This chapter deals with effective drug designing, including the structure-activity relationship and the influence of various functional groups on the activity of a drug compound. The toxicological impact of drugs on the environment has also been explored. In recent times, it has been successfully studied that residue of drugs could enter the ecosystem through the water channel. It directly or indirectly impacts soil, groundwater, and surface water, and creates environmental and health problems.

Keywords: Drug, Environment, Functional group, Organic, Stereochemistry, Therapeutic, Toxicological.

[*] **Corresponding author Musheer Ahmad:** Department of Applied Chemistry, Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, India; E-mail: amusheer4@gmail.com

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