



COVID-19:
ORIGIN, IMPACT AND MANAGEMENT
PART 2



Editors:
Tahmeena Khan
Alfred J. Lawrence

Bentham Books

COVID-19: Origin, Impact and Management (Part 2)

Edited by

Tahmeena Khan

*Department of Chemistry
Integral University, Lucknow
India*

&

Alfred J. Lawrence

*Department of Chemistry
Isabella Thoburn College, Lucknow
India*

COVID-19: Origin, Impact and Management (Part 2)

Editors: Tahmeena Khan & Alfred J. Lawrence

ISBN (Online): 978-981-5165-94-4

ISBN (Print): 978-981-5165-95-1

ISBN (Paperback): 978-981-5165-96-8

© 2023, Bentham Books imprint.

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

First published in 2023.

CONTENTS

FOREWORD I	i
FOREWORD II	ii
PREFACE	iii
LIST OF CONTRIBUTORS	iv
CHAPTER 1 COVID-19 PANDEMIC: OUTBREAK, EPIDEMIOLOGY AND IMMUNOLOGY	1
<i>Uzma Afreen, Ushna Afreen and Daraksha Bano</i>	
INTRODUCTION	1
HISTORICAL PERSPECTIVE	3
Origination of COVID-19 and Statistical Data	3
Morphological Features of SARS-CoV-2	4
The Structural Proteins:	5
Current Situation of COVID-19 all over the World	5
Mode of Infection	6
Mode of Transmission	7
Measures to Contain COVID-19	8
Diagnosis	9
1. NAATs (Nucleic acid Amplification Tests)	9
2. Antigen Test	9
3. Self-Tests	9
PREVENTION	10
1. General Measures	10
2. Measures adopted by Governments all over the world	10
Probable Medicinal Intervention	11
Antiviral Drugs	11
Antibacterial Drugs	12
Antimalarial Drugs	13
Immunomodulatory Drugs	13
Monoclonal Antibodies	13
Drug Repurposing and Computational Assessment	13
Vaccines and Futuristic Strategies	14
RNA-Based Vaccines	15
Viral Vector Vaccines	15
Protein-Based Vaccines	15
Inactivated Virus Vaccines	15
COVID-19 Vaccines for Children	16
CONCLUSION	17
CONSENT FOR PUBLICATION	18
CONFLICT OF INTEREST	18
ACKNOWLEDGEMENTS	18
REFERENCES	19
CHAPTER 2 THE IMPACT OF AIR POLLUTION AND ENVIRONMENTAL FACTORS ON COVID-19 TRANSMISSION	22
<i>Alfred J. Lawrence, Vinay P. Aneja and Tahmeena Khan</i>	
INTRODUCTION	23
HISTORICAL PERSPECTIVE	23
Facts and Figures	24
Structure and Activity Domain of SARS-CoV-2	25

The Search for Possible Medicinal Interventions	26
Mode of Spread	26
Respiratory Transmission	26
Transmission through Direct Contact	27
Transmission through Domestic Pets	27
Vertical Transmission	27
Faecal–Oral (or Fecal Aerosol) Transmission	27
Clinical Symptoms with Special Emphasis on Respiratory Functionalities	27
AIR POLLUTION AS A CONTRIBUTING FACTOR	28
Studies Suggesting an Alleged Association between Air Quality and COVID-19	29
Is Indoor Air Pollution Neglected Here?	31
Pathophysiology of SARS-CoV-2 and Similarity in Mechanistic Action with Particulate Matter	31
Household Characteristics and their Impact	32
Improvement in Air Quality during the Lockdown: Exploring the Positive Aspect of the Pandemic	33
Contribution of Meteorological Parameters	34
Natural Resources as Immunity Boosters- A Probable Preventive Measure	35
CONCLUSION	36
CONSENT FOR PUBLICATION	37
CONFLICT OF INTEREST	37
ACKNOWLEDGEMENT	37
REFERENCES	37
CHAPTER 3 IMPACT OF THE COVID-19 PANDEMIC: A CHANGED WORLD	44
<i>Umang Tandon and Apoorva Tandon</i>	
INTRODUCTION	44
THE CORONAVIRUS CURVES	45
ECONOMIC IMPACT	46
Effect on the Global Supply Chain	48
Effect on Employment and Workforce Disparities	49
Effect on Tourism and Hospitality	53
Effect on the IT Industry	54
CONCLUSION	55
CONSENT FOR PUBLICATION	55
CONFLICT OF INTEREST	55
ACKNOWLEDGEMENT	55
REFERENCES	56
CHAPTER 4 IMPACT OF COVID-19 PANDEMIC ON WOMEN	57
<i>Tahmeena Khan, Saima Arif and Alfred J. Lawrence</i>	
INTRODUCTION	57
COVID-19 and its Impact	58
Effect of COVID -19 Pandemic on the Human Race	60
Women and COVID 19	60
Women and Health and Hygiene	61
Reproductive Health	62
Psychological Health	62
Nutritional Aspects Concerning Women’s Health	63
The Impact of the Pandemic on Indian Women	64
A SURVEY-BASED STUDY WITH WOMEN	66
RESULTS AND DISCUSSION	66

Demographic Details	66
Employment Details	68
Physical Fitness and Nutritional Aspects	68
Sanitary and Hygiene Practices	70
CONCLUDING REMARKS	74
CONSENT FOR PUBLICATION	74
CONFLICT OF INTEREST	74
ACKNOWLEDGEMENT	74
REFERENCES	74
CHAPTER 5 VACCINATION HESITANCY AND ADAPTATION WITH PARTICULAR EMPHASIS ON WOMEN	78
<i>Tahmeena Khan, Alfred J. Lawrence, Amos Nascimento and Rohan Srivastava</i>	
INTRODUCTION	79
A QUESTIONNAIRE-BASED STUDY	81
RESULTS AND DISCUSSION	82
Demographic Details	82
COVID-19 Vaccine Awareness	82
Safety Concerns Related to Vaccination	85
Misconceptions and Disbeliefs	88
CONCLUSION	93
CONSENT FOR PUBLICATION	93
CONFLICT OF INTEREST	93
ACKNOWLEDGEMENT	93
CHAPTER 6 COMPUTATIONAL DRUG DISCOVERY AGAINST COVID-19	96
<i>Shristi Modanwal, Viswajit Mulpuru and Nidhi Mishra</i>	
INTRODUCTION	96
VIRTUAL SCREENING METHODS	98
Structure-Based Virtual Screening	99
<i>Protein-Ligand Docking</i>	99
<i>Structure-Based Pharmacophores</i>	101
Ligand-Based Virtual Screening	101
<i>Similarity Method</i>	102
<i>Pharmacophore Mapping</i>	103
<i>Machine Learning Method</i>	104
Combined LBVS and SBVS	105
INTERPRETING DRUG INTERACTION	105
APPLICATION OF VIRTUAL SCREENING FOR COVID 19 THERAPEUTICS	106
FUTURE PROSPECTS OF VIRTUAL SCREENING	106
CONCLUSION	106
CONSENT FOR PUBLICATION	107
CONFLICT OF INTEREST	107
ACKNOWLEDGEMENT	107
REFERENCES	107
CHAPTER 7 METHODS IN DRUG REPURPOSING: EMPHASIS ON COVID-19	111
<i>Akhilesh Kumar Maurya and Nidhi Mishra</i>	
INTRODUCTION	111
Drug Repurposing Methods	112
Computational Methods	113
<i>Structure-Based</i>	113

Artificial Intelligence-Based	114
Pathway-Based and Genetic Associations	114
Experimental Approaches	115
<i>Targeted Based Approaches</i>	115
<i>SARS-CoV-2 Drug Repurposing</i>	115
Drug Repurposing Molecules for COVID-19	116
<i>Remdesivir</i>	116
<i>Ribavirin</i>	117
<i>Darunavir</i>	117
<i>Chloroquine</i>	118
<i>Hydroxychloroquine</i>	119
<i>Dexamethasone</i>	119
<i>Emapalumab and Sarilumab</i>	120
Computational Study	120
CONCLUSION	121
CONSENT FOR PUBLICATION	122
CONFLICT OF INTEREST	122
ACKNOWLEDGEMENTS	122
REFERENCES	122
CHAPTER 8 VIRTUAL SCREENING OF PHYTOCHEMICALS IN SEARCH OF A POTENTIAL DRUG CANDIDATE FOR COVID-19: DFT STUDY AND MOLECULAR DOCKING	127
<i>Nikita Tiwari, Lubna Jamal and Anil Mishra</i>	
INTRODUCTION	127
MATERIALS AND METHODS	130
DFT Calculations	130
Molecular Docking	131
RESULT AND DISCUSSION	131
DFT Calculation Studies	131
Thermodynamic Properties	131
Molecular Orbital Properties	134
Binding Affinity and Binding Interactions Analysis	136
CONCLUSION	141
CONSENT FOR PUBLICATION	142
CONFLICT OF INTEREST	142
ACKNOWLEDGEMENTS	142
REFERENCES	142
CHAPTER 9 ROLE OF IMMUNITY AGAINST COVID-19	145
<i>Nidhi Singh</i>	
INTRODUCTION	145
Immune System: Process and Defense	146
Creation of Barriers for the Prevention of Pathogens	146
Identification of Pathogens After their Entry	147
Elimination of Pathogens	148
Generation of Immunological Memory	148
STRUCTURE OF SARS-COV-2	149
Immunopathogenesis of COVID-19	150
Non-Severe Stages	151
Severe Stage	151
NUTRITION AND IMMUNITY	151

Vitamin A and Immunity Efficiency	152
Vitamin C and Immunity Efficiency	152
Vitamin D and Immunity Efficiency	153
Zinc Micronutrient and Immunity Efficiency	153
Copper Micronutrient and Immunity Efficiency	154
HERD IMMUNITY AND CORONAVIRUS	154
NATURAL PRODUCTS AND IMMUNITY AGAINST COVID-19	154
Tulsi as Immunity Booster	155
Giloy as Immunity Booster	155
Ashwagandha as Immunity Booster	156
Dalchini as Immunity Booster	156
Sunthi as Immunity Booster	157
Marich as Immunity Booster	157
VACCINATION AND IMMUNITY AGAINST COVID-19	157
CONCLUSION	158
CONSENT FOR PUBLICATION	159
CONFLICT OF INTEREST	159
ACKNOWLEDGEMENTS	159
REFERENCES	159
SUBJECT INDEX	165

The Impact of Air Pollution and Environmental Factors on COVID-19 Transmission

Alfred J. Lawrence¹, Vinay P. Aneja² and Tahmeena Khan^{3,*}

¹ Department of Chemistry, Isabella Thoburn College, Lucknow, India

² North Carolina State University, USA

³ Department of Chemistry, Integral University, Lucknow, India

Abstract: SARS-CoV-2 (COVID-19) has caused serious mortal damage to the human race. The virus causes respiratory infections, and many studies are trying to comprehend the mode of spread and infection. This chapter has explained the origin of the virus, its structure and activity domain, symptoms, medicinal interventions, and particularly various modes of spread with emphasis on air pollution as contributing and facilitating factors assisted with favourable meteorological conditions, including temperature and relative humidity. Pieces of evidence from different countries suggest that the spread of the virus may be facilitated by air pollution and people who are exposed to high pollution levels are more susceptible to falling victim to the virus. Transmission of the SARS-CoV-2 may be facilitated by the airborne particulate matter, and both particulate matter and coronavirus cause oxidative stress in the body that helps in enhancing the susceptibility and severity towards respiratory infection. Not only ambient air pollution, but indoor air pollution (IAP) is also a factor worth considering. People in developing and under-developed nations are at high risk as they are exposed to high IAP levels. Awareness must be created to educate them about the associated harmful consequences, including the risk of catching the lethal COVID-19 infection. In the absence of any concrete medicinal solution, it is necessary to build immunity which may be uplifted by the usage of natural food sources, including herbs and spices. An overview of some commonly available herbs and spices of medicinal importance has also been given in the chapter.

Keywords: Air Pollution, Airborne, Environment, Humidity, Indoor Pollution, Oxidative Stress, Particulate matter, Respiratory Infection, SARS-CoV-2, Temperature.

* Corresponding author Tahmeena Khan: Department of Chemistry, Integral University, Lucknow, India; E-mail: tahminakhan30@yahoo.com



Tahmeena Khan

Dr. Tahmeena Khan is currently working as an assistant professor, in the Department of Chemistry, Integral University. She did M.Sc., and holds a specialization in inorganic chemistry. She did her M.Phil. in magnetic resonance spectroscopy and magnetic resonance imaging and worked on automated 3D structure determination of proteins for her dissertation. For her doctoral degree, she worked on mixed ligand-metal and mixed metal-ligand complexes of thiosemicarbazones and their therapeutic properties. She holds fifteen years of teaching experience and has published more than forty research papers and twenty book chapters. She also has two international books and two national books as editor and two books as author to her credit. Dr. Khan is also a life member of several academic bodies. She has keen interest in medicinal and environmental chemistry.



Alfred J. Lawrence

Dr. Alfred J. Lawrence is working as Assistant Professor in the Department of Chemistry, Isabella Thoburn College, Lucknow. He is also serving as the coordinator of the Research & Networking Cell and the chairperson of the Internal Quality Assurance Cell (IQAC) of the college. He holds twelve years of teaching experience and twenty years of research experience in Air Pollution monitoring and Health Risk Assessment. He has done his Ph.D. from St. John's College, Agra and holds four years of Post-Doctoral research experience from Purdue University, USA. He has been a visiting scholar to the University of Manchester and Oxford University, UK. He has published more than thirty five research papers in reputed international journals and five book chapters. He has also edited two international books and two conference proceedings. He has completed two research projects and is currently working on a project funded by the Department of Higher Education, Govt. of Uttar Pradesh. He has received many fellowships and was awarded International Society of Indoor Air Quality (ISIAQ) Fellowship, ETH Fellowship and International Society for Environmental Epidemiology Fellowship, Department of Science & Technology Travel Grant, University Grant Commission Travel Grant to present Research work in Ghent University, Belgium; ETH University, Switzerland; ISEE - Italy, University of Scotland, England and AWMA, USA respectively to present his research work.