



COVID-19:
ORIGIN, IMPACT AND MANAGEMENT
PART 2



Editors:
Tahmeena Khan
Alfred J. Lawrence

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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*

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Editors: Tahmeena Khan & Alfred J. Lawrence

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FOREWORD I

I feel it a pleasure to write forward to the book titled “COVID-19: Origin, Impact and Management” edited by Dr. Alfred Lawrence and Dr. Tahmeena Khan. The SARS-CoV-2 or COVID-19 pandemic has jolted the entire world at different levels. It is not only the health sector that has been greatly impacted, but human life has suffered at multi-levels, be it psychological well-being, economic upheaval or discrimination in caregiving at home as faced by women. The education sector also saw reform as online mode took over. The situation is more severe and grim in developing countries and it is very important to find out the vulnerable groups, having access to lesser means of protection and prevention.

This innovative book is an interesting reading material as the assorted chapters cater to different aspects related to the pandemic. Several interesting case studies are conducting an in-depth analysis of the impact of the COVID-19 outbreak on different target groups. The management strategies and vaccine development have also been nicely explained. The interdisciplinary nature of the book makes it suitable for academicians and students belonging to science, humanities, and commerce background. The chapters are very well written and presented in an easy-to-understand manner.

Ajay Taneja
Department of Chemistry
Dr. B. R. Ambedkar University
Agra – Uttar Pradesh
India

FOREWORD II

It gives me immense pleasure to introduce the second part of the book **COVID-19: Origin, Impact and Management** ably edited by Dr. Tahmeena Khan and Dr. Alfred J. Lawrence. The book has covered many important aspects related to the COVID-19 mayhem which claimed millions of lives world over. The second part of the book has shed light on many important aspects like the effect of the pandemic on women and how they are adapting to the change in lifestyle. Not only this, but the book also includes chapters on computational drug discovery which may be useful to researchers working in medicinal chemistry. The chapters are composed and selected very ably and the authors have done a great job as all the chapters are well-written, informative and present facts in a beautiful manner.

I wish the editor great success and hope the readers would be benefitted from the enriching book.

S. H. Hasan
Department of Chemistry
IIT (BHU) Varanasi– Uttar Pradesh
India

PREFACE

The emergence of the COVID-19 pandemic was an unprecedented situation that impeded the physical and mental well-being of people globally. The expeditious discovery of vaccines and medication for decelerating the spread of SARS-CoV-2 catered to alleviating mortality rates. A comprehensive discussion on the pandemic and its impact on billions of lives has been done in part one of the two books. This part provides a meticulous overview of the COVID-19 pandemic. This book intends to collaboratively serve students, scientists and academicians from different academic areas such as science, humanities, economics; and even common masses. The collation of various heads in this book is based on contemporary needs and elaborately gives an insight into the pandemic, its impact on people's lives, especially on women, the variations that it brought in the world, and the role of air quality in exacerbating the disease. Drug discovery and vaccination hesitancy-related challenges are also scrupulously described in this book. Authors from various eminent institutions have contributed to the book which makes it a valuable collection of information. Computational Drug Discovery against the pandemic, DFT studies and molecular docking, and drug repurposing for searching potential drug candidates are the highlights of the book. Special emphasis is laid on the impact of the COVID-19 pandemic on women. The book vouches to provide a deep insight into the outbreak, epidemiology, immunology and management of SARS-CoV-2 and will be valuable for evolutionary biologists, pharmaceutical scientists and doctors. In essence, the book will supply a plethora of relevant information for degree students, research scholars, academicians, scientists and anyone who finds an interest in gathering information about the disease.

Tahmeena Khan

Department of Chemistry
Integral University
Lucknow
India

&

Alfred J. Lawrence

Department of Chemistry
Isabella Thoburn College
Lucknow
India

List of Contributors

Alfred J. Lawrence	Isabella Thoburn College, Lucknow, India
Akhilesh Kumar Maurya	University of Lucknow, Lucknow, India
Anil Mishra	University of Lucknow, Lucknow, India
Amos Nascimento	University of Washington, Tacoma/Seattle, USA
Apoorva Tandon	Krishna Institute of Engineering and Technology, Group of Institutions, Ghaziabad, India
Daraksha Bano	Integral University, Lucknow, India
Lubna Jamal	University of Lucknow, Lucknow, India
Nidhi Mishra	Indian Institute of Information Technology, Prayagraj, India
Nidhi Singh	Isabella Thoburn College, Lucknow, India
Nikita Tiwari	University of Lucknow, Lucknow, India
Rohan Srivastava	Integral University, Lucknow, India
Saima Arif	CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow, India
Shristi Modanwal	Indian Institute of Information Technology, Prayagraj, India
Tahmeena Khan	Integral University, Lucknow, India
Umang Tandon	Isabella Thoburn College, Lucknow, India
Ushna Afreen	Department of Chemistry, Lucknow University, Lucknow-226007, India
Uzma Afreen	University of Lucknow, Lucknow, India
Vinay P. Aneja	North Carolina State University, USA
Viswajit Mulpuru	Indian Institute of Information Technology, Prayagraj, India

CHAPTER 1

COVID-19 Pandemic: Outbreak, Epidemiology and Immunology**Uzma Afreen¹, Ushna Afreen¹ and Daraksha Bano^{2,*}**¹ *Department of Chemistry, Lucknow University, Lucknow-226007, India*² *Department of Chemistry, Integral University, Lucknow-226026, India*

Abstract: The SARS-CoV-2 virus-led COVID-19 pandemic jolted the whole world at different levels. Severe acute respiratory syndrome (SARS) caused death in severe cases leading to millions of mortalities. This chapter attempts to present an overview of the whole fiasco created by the spread of the virus along with the historical background, structural features and important proteins of the virus, modes of infection and transmission and different diagnostic means like viral and antibody tests. The authors have presented the latest statistical data on the number of cases and mortalities reported across the globe and also elaborated on the probable remedial interventions like the different antiviral, antimalarial drugs which are being explored for treatment and also explored the utility and applications of drug repurposing and computational strategies for drug development. The authors have also elaborated on the different vaccines developed to curb the disease and explained the development of COVID-19 vaccines for children. Overall the chapter has summarized key facts associated with COVID-19 in a nutshell and it may prove beneficial to the readers to understand the disease more clearly.

Keywords: ACE-2, Envelope Protein, Gag-Pol Polyprotein, MERS, NAAT, Nucleocapsid Protein, OTC Tests, RT-PCR, RdRp, SARS-CoV-2, SARS, Spike Protein.

INTRODUCTION

The outbreak of the SARS-CoV-2 or COVID -19 virus has led to one of the worst pandemics in recent times. Coronaviruses (CoVs) have been recognized for over 50 years. The virologists derived the word “corona” from the sun comparing the characteristic projections on the surface of the virus with the solar corona. CoVs cause severe acute respiratory syndrome (SARS) which may lead to death in severe cases. These viruses chiefly infect human and non-human mammals and birds [1]. Coronaviruses are included in the subfamily Coronavirinae, in the

* **Corresponding author Daraksha Bano:** Department of Chemistry, Integral University, Lucknow-226026, India; E-mail: darakshab@iul.ac.in.

family Coronaviridae of the order Nidovirales [2]. Based on their phylogeny and genotype, this subfamily consists of four genera—Alphacoronavirus, Betacoronavirus, Gammacoronavirus and Deltacoronavirus. The alphacoronaviruses and betacoronaviruses infect only mammals, while the gammacoronaviruses and deltacoronaviruses chiefly infect birds, although some of them can also infect mammals [3]. Coronaviruses are single positive-sense RNA viruses which show greater mutation rates as compared to DNA viruses, owing to which they have better adaptation for survival. CoVs mainly affect birds and mammals. Before 2019, there were only six CoVs that were known to infect humans and caused respiratory diseases *viz.* HCoV-229E, HCoV-OC43, HCoV-NL63, HKU1, SARS-CoV and MERS-CoV. Among these, SARS-CoV and MERS-CoV have been reported to cause a severe respiratory syndrome in humans. MERS (Middle East respiratory syndrome) was first reported in Saudi Arabia in the year 2012. The COVID-19 virus, the causative agent for the coronavirus disease outbreak in 2019 emerged in Wuhan, Hubei Province, China. Wuhan, the epicentre of this virus, reported its first case in 2019. It was called Wuhan Novel Coronavirus (2019-nCoV). On the 31st of December 2019, the Chinese authorities alerted the World Health Organization (WHO) of a series of cases having pneumonia-like symptoms in the city of Wuhan. Shortly after the alert, it was recognized that the infections in humans likely originated from Huanan Seafood Market in Wuhan. After about two weeks, a team of Chinese scientists in collaboration with WHO announced that a new coronavirus (2019-nCoV), identified through genomic sequencing, was the causative agent of this pneumonia-like disease that originated in Wuhan [2]. On 9th January 2020, China declared that a novel coronavirus is the causative agent of this coronavirus disease outbreak in 2019 which is now known as COVID-19 [1]. This novel coronavirus named the severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2 or 2019-nCoV) radiated from Wuhan to other areas of China. It was found to possess high homology (~80%) to the SARS-CoV [4]. The virus that causes COVID-19 (SARS-CoV-2) is identified to originate in bats from where it spread to humans through contamination of meat sold in Wuhan's meat markets with wild animals' wastes [1]. By January 7th 2020, a novel beta coronavirus, SARS-CoV-2, was identified. Mortality rates are higher among people over 60 years of age and with pre-existing medical problems such as hypertension, diabetes and cardiovascular disease [5]. COVID-19 represents a spectrum of clinical manifestations encompassing fever, dry cough, fatigue and other pneumonia-like symptoms. SARS-CoV-2 is highly contagious. The mode of transmission of the disease is droplet infection and direct contact. Although respiratory droplet and contact transmission are the main transmission routes for the spread of SARS-CoV-2, aerosol and faecal-oral transmissions might also be responsible for its transmission, but have not been confirmed yet [6, 7].

HISTORICAL PERSPECTIVE

Origination of COVID-19 and Statistical Data

The ability of viruses to evolve quickly and unpredictably as they can mutate rapidly has posed great challenges to virologists. Their erratic behaviour has attracted researchers to understand their evolutionary modalities and develop strategies to subdue their activity. Many viruses have been causing various diseases in living organisms and have been, modifying their genome *via* mutation. This originates a need for continuous research on different viruses. Human viruses are distinguished based on their physical, chemical and biological properties into 26 distinct families. Coronaviridae is one of these families which includes highly infectious viruses which were earlier known to cause mild intestinal and respiratory infections in animals and humans. In the year 2002-2003, a very severe and fatal respiratory disease was encountered in Guangdong, China known as SARS which proved to be fatal. After a gap of nearly ten years another related and highly infectious strain, MERS originated in middle eastern countries where the first case was reported in the year 2012 in Jeddah, Saudi Arabia to be caused due to MERS-CoV (Middle East respiratory syndrome- coronavirus) [8]. Humans are highly susceptible to SARS-CoV and MERS-CoV (betacoronaviruses) which cause severe respiratory complications in humans. Other human coronaviruses cause mild upper respiratory tract infections with mild symptoms in adults these include HCoV-NL63, HCoV-229E, HCoV-OC43 and HKU1. Infants, elderly people and immunocompromised people (people with the impaired immune system) are susceptible to all the above types of human coronaviruses [3].

Later in December 2019 another fatal strain of Coronavirus came into existence in Wuhan City, China. It was named COVID-19 as it was first reported in the year 2019 [3]. A timeline of pandemics caused due to CoVs is represented in Fig. (1).

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

INTRODUCTION

The outbreak of Severe Acute Respiratory Syndrome coronavirus (SARS-CoV-2) has surfaced as a major health concern all over the world [1]. The outbreak was pronounced a health emergency on 30th January 2020, and subsequently, on 11 March 2020, the WHO declared COVID-19 a pandemic. The coronavirus was first isolated in the year 1965 by Tyrrell and Bynoe from a child with a cold and flu and termed B814 [2]. The term coronavirus was coined owing to the morphological characteristics of the virus in the year 1968 [3]. The virus may be transmitted through, 1) direct contact with the infected person, 2) aerosol generation and inhalation by a healthy person and 3) environmental factors [4]. It has been found that dried SARS-CoV-2 can be viable for 3-4 days at room temperature between 22-25 °C for 14 days at a temperature of 4 °C but becomes inactive at a warm temperature. The live virus has been cultured from aerosols and surfaces even after hours of inoculation, but strong evidence suggests respiratory transmission with closeness to the infected patient and ventilation being the key determinants [5]. The viral spike protein (S) binds to the angiotensin-converting enzyme 2 (ACE2) receptor, which is crucial for the entry of the pathogen into the host cell and the distribution of ACE2 [6]. The viral load is highest in the upper respiratory tract initially and later on reaches the lower respiratory tract (sputum). It has also been found that susceptibility to infection increases with age [7]. A study from Iceland reported 6.7% and 13.7% positivity in children and adults, and 4% and 17.1% positivity was obtained from Wuhan, China [8]. Low expression of ACE2 in children may be responsible for the difference in positivity rate [9].

HISTORICAL PERSPECTIVE

The novel coronavirus that causes COVID-19 has been linked to animals and was reportedly transmitted to humans in Wuhan, China, in December 2019 [10]. To date, all coronaviruses causing human infection originated from bats or rodents [11]. In the year 2007, scientists from Hong Kong brought to notice the emergence and re-emergence of SARS [11]. The US Centers for Disease Control and Prevention (2017) estimates that three-quarters of new or emerging diseases that infect humans originate in animals [12]. Outbreaks of previously known SARS-CoV and MERS-CoV involved exposure to other animals like civet cats and dromedary camels. The virus appears as a crown with petal-like projections protruding from the surface, thereby acquiring the Latin name “corona” meaning crown [13]. They are positive-sense RNA viruses belonging to the Coronavirinae subfamily of the order Nidovirales [14] and are categorized as alpha, beta, gamma and delta based on their genomic structure. Out of which, the first two cause respiratory symptoms in mammals [15].

Two major outbreaks caused by coronaviruses, 1- SARS in 2003 caused 1,000, and 2- Middle East Respiratory Syndrome (MERS) in 2012 led to 862 fatalities. The SARS incidence was first reported in late 2002 and reemerged in late 2003 [16] due to an interspecies transmission. The viral outbreak was first reported in China, where the increasing demand for animal proteins, including civets, led to their bearing in close confinements, and in the absence of biosafety measures, the virus spread like an epidemic from animals to humans, later from person to person transmission [17]. The virus is zoonotic because of its transmission from animals to humans [18]. The SARS coronaviruses are characterized by spike proteins containing a variable receptor-binding domain (RBD) which binds to the ACE-2 receptor [19], facilitating viral entry in the target cells. The RBD of SARS-CoV-2 seems to be a mutant of RaTG13, a virus sampled from bats [20], thereby showing that the virus originated from bats. Until December 2019, six coronaviruses were identified to cause infection in humans. HCoV-NL63, HCoV-229E, HCoV-OC43 and HKU1 were responsible for causing mild cold-type symptoms in people with compromised immunity, and the other two led to pandemics during the last two decades.

Facts and Figures

WHO has characterized the transmission as 1- Nations with no reported cases, 2- Infrequent cases, 3-Clusters of cases, 4- Community transmission [20]. From 31st December 2019 to 21st January 2022, 340543962 cases have been reported with 5570163 casualties (European Centre for Disease Prevention and Control (ECDC) 2022). With time, the virus changes its properties like the spread, severity of infection, therapeutic interventions, diagnostic methods and other public health measures. WHO has been in the process of assessing the evolution of SARS-CoV-2 since January 2020 and characterized Variants of Interest (VOIs) and Variants of Concern (VOCs) to guide comprehensive research. The changes can be monitored by monitoring changes in amino acid substitutions to inform countries about changes that may be needed to respond to the variant. Different countries may also report and designate other variants which are found in the patients. To contain the transmission through proven disease control measures and avoiding transmission to animal populations are important methods to decrease the chances of mutations having harmful health impacts. Research so far indicates that the general health and social measures and infection deterrence and management measures have been effective against COVID-19-related hospitalization and deaths. Table 1 summarizes the known variants of SARS-CoV-2.

Impact Of The COVID-19 Pandemic: A Changed World

Umang Tandon^{1,*} and Apoorva Tandon²

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

² Department of Computer Science, Krishna Institute of Engineering and Technology, Group of Institutions, Ghaziabad, India

Abstract: Coronavirus disease-2019 (COVID-19) is predicted to have long-term consequences on the world's physical, mental and economic levels. June 2020 Global Economic Prospects describe the immediate and near-term impact of the pandemic, additionally the long-term injury to growth prospects. The baseline forecast predicts a 5.2% contraction in world GDP, despite the efforts made by governments to combat the downswing aided by business and financial support. Half the world's 3.3 billion personnel are threatened by the loss of their jobs. Moreover, workers within the informal economy are significantly vulnerable as a result of the lack of social protection, access to quality health care and productive assets. Individuals are finding it troublesome to survive through imprisonment as a result of a lack of resources to earn a living. According to Moody, the economic impact of the recent increase in COVID-19 cases is going to be restricted from April to June quarter, with a robust rebound within the last half of the year. The slower growth rate, on the other hand, can impede near-term economic recovery and have an impression on long-term growth dynamics. This study is focused on determining the critical effects of a Coronavirus pandemic on the global economy and anticipating the scenario that would confront the global economy soon. This research examines the various elements of Coronavirus and its economic implications.

Keywords: COVID-19, GDP, Global Economy, Global Supply Chain, Growth, Market Charge, Pandemic, Productivity, Recovery.

INTRODUCTION

The 1918 Spanish influenza, HIV/AIDS outbreaks, SARS (Severe Acute Metabolic Process Syndrome), MERS (Middle East Metabolic Process Syndrome) and Ebola are all epidemics that have unfolded throughout human history. COVID-19 was designated a global health emergency by the World Health

* Corresponding author Umang Tandon: Department of Commerce, Isabella Thoburn College, Lucknow, India; E-mail: umangtandon2311@gmail.com

Organization in January 2020 and a pandemic on March 11, the highest grade of medical crisis [1]. Since then, the situation has escalated into a worldwide public health and economic calamity, with far-reaching consequences for the world's \$90 trillion economies not seen in almost a century. In a take on the John Donne poem, "No Man is an Island," the viral illness spread through and across countries and touched nearly every community, highlighting the global economy's interconnected nature. In March 2020, the epicentre of transmissions had moved from China to Europe, mainly Italy, but by April, the focus switched to the United States, where infection rates escalated manifold. By April 2021, viral hotspots had arisen in India, Brazil, and parts of Africa and Asia, with infection and fatality rates reaching new highs [2].

In the shortterm, every country's healthcare system has a limited capacity of ICUs, hospital beds, number of medics and paramedics, ventilators, *etc.* This puts a limit on the number of patients who can be treated successfully. Flattening the infection curve, that is, reducing the incidence of contamination and infections, is crucial to preventing clinical hospital capacity overflow in third-world countries, as well as the mortality toll that entails. When a considerable proportion of the population lives in slums, social distancing regulations become more difficult to apply, making it more difficult to control the spread. While high-income nations have an average of more than four hospital beds per thousand inhabitants, low-income countries have as few as 0.5, making it all the more difficult to treat critically ill patients [3]. This factor made coronavirus a major threat to developing countries.

THE CORONAVIRUS CURVES

The pandemic curve (Fig. 1) also promotes a recession curve (Fig. 2), which must also be addressed. The impacts of the disease are disruptive, and they may leave scars that prevent the economy from returning to its pre-shock state. While doing nothing damages demand and supply, social-distancing policies have exacerbated the problem [3]. Even though some people can work from home, they only make up a small percentage of the entire workforce. The masses whose income is dependent on their physical mobility are disproportionately affected by lockdowns and social isolation regulations. Another problem arises from the informality of labour in emerging countries, where the shadow economy accounts for 50% to 90% of total employment. Welfare benefits, health insurance, and paid holidays are not available to informal workers. Due to this informality of work, policies aiming at formal work, such as expanding unemployment insurance, lowering payroll taxes, and extending paid medical leave, leave a limited impact on the overall economy [3].

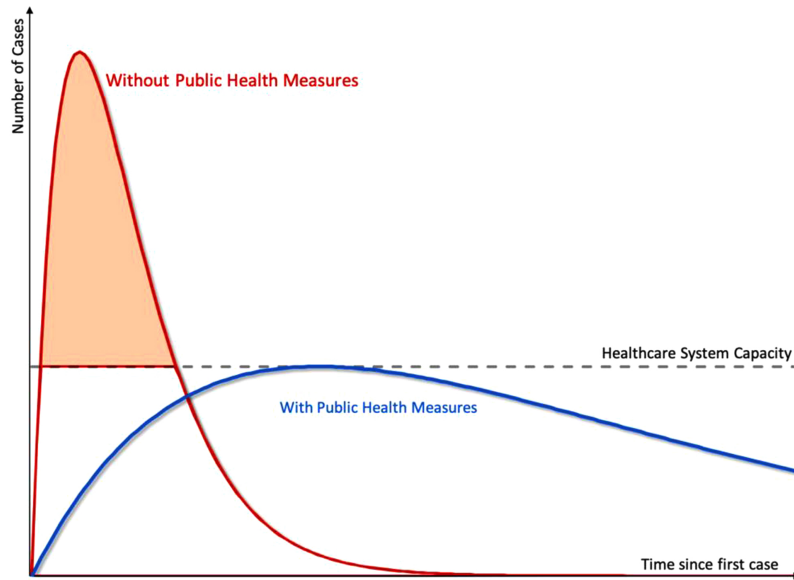


Fig. (1). The Pandemic Curve [Source: Gourinchas (2020)].

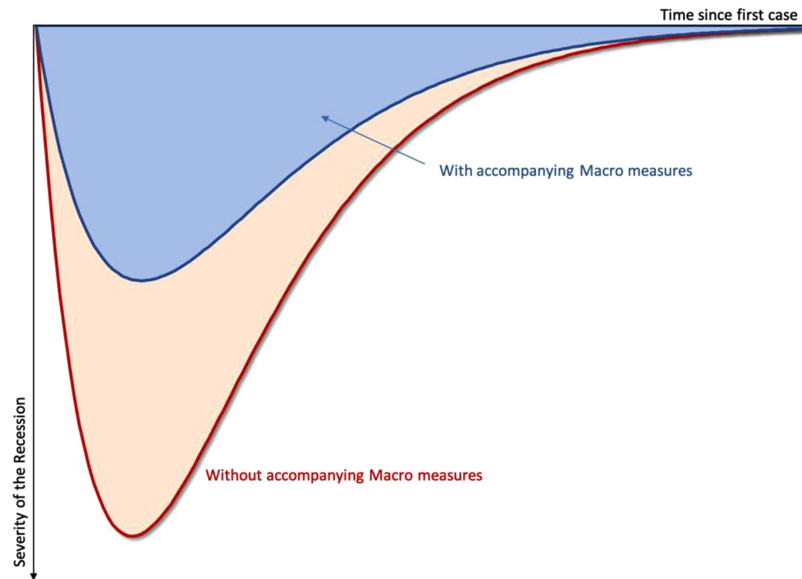


Fig. (2). The Recession Curve [Source: Gourinchas (2020)].

ECONOMIC IMPACT

Since the outbreak, the effects of the disease have been felt beyond mortality and morbidity in the present-day strongly connected world [4]. This has already been

Impact of COVID-19 Pandemic on Women

Tahmeena Khan¹, Saima Arif^{2,3} and Alfred J. Lawrence^{2,*}

¹ Department of Chemistry, Integral University, Lucknow, 226026, U.P., India

² Department of Chemistry, Isabella Thoburn College, Lucknow, 226007, Uttar Pradesh, India

³ Toxicokinetics Laboratory, CSIR- Indian Institute of Toxicology Research (IITR), Lucknow, 226001, Uttar Pradesh, India

Abstract: SARS-CoV-2 virus, leading to the COVID-19 pandemic, was first recognized in 2019. The impact of the crisis is never gender-neutral, and COVID-19 is no exception. While everyone is facing unprecedented challenges, women bear the brunt of the economic and social fallout of COVID-19. Hygiene and nutritional aspects are important parameters for the assessment of the overall health and well-being of a person. This chapter has shed light on the impact of the COVID-19 pandemic on women and how their sanitary/hygiene routine has been impacted in the current scenario. Through an online questionnaire survey with 510 women, the overall impact on their lives, including health and hygiene and nutritional practices, is presented as a case study. 69.4% of women reported spending some time on a physical fitness regime, and 66.2% of them believed that wearing a mask can reduce the risk of infection. 56.3% of women reported no side effects related to masks, however, 25.6% of women reported breathing issues whereas, skin rashes and itching and ear pain were some other symptoms reported. Women became more careful about their health during the pandemic, and 73.1% of them reported to have consumed additional measures to boost their immunity, and 74.4% of the women reported that their fruit intake increased during the pandemic. 52.2% of the respondents also reported consuming some health supplements. The awareness can be linked to educational status as the majority of respondents had university degrees, out of which 33.5% were graduates, and 30% were post-graduates.

Keywords: COVID-19, Education, Health, Helsinki Declaration, Hygiene, Immunity, Nutrition, Physical fitness, Protection, Survey, Women.

INTRODUCTION

The novel coronavirus (COVID-19) or SARS-CoV-2 pandemic started in Wuhan, China, at the end of 2019 and spread over the world by 2020. In the absence of

* Corresponding author Alfred J. Lawrence: Department of chemistry, Isabella Thoburn College, Lucknow-226007, Uttar Pradesh, India: E-mail: Alfred_lawrence@yahoo.com

any concrete medicinal solutions, various preventive measures like social distancing and massive lockdowns have been implemented by governments, resulting in people staying at home. The lockdowns also saw closures of educational institutions, offices, gyms and other non-essential services [1]. The pandemic has not only posed a threat to human health, but it has also had an impact on human existence at all levels, resulting in economic losses and jeopardising mental health. The current situation's societal impacts are partly discriminatory and gender prejudiced, notably affecting the marginalised population and women. The “care economy” has been severely disrupted, rendering women more vulnerable to bear the effects of the situation not just now, but also in the near future [2]. Gender is a social predictor of health [3], and women report more unhealthy days on average, both emotionally and physically, than males [4]. Asthma, diabetes, and myocardial infarction are examples of health issues.

Health conditions like asthma, diabetes and myocardial infarctions [5] are often encountered by women, particularly those belonging to less privileged socioeconomic classes, and those belonging to the rural background and low educational profiles [6]. The coronavirus pandemic is expected to plunge 47 million women into poverty, according to United Nations research. According to the report, while the pandemic will have a worldwide impact on poverty, it will disproportionately affect women. By 2021, there will be 118 women for every 100 men aged 25 to 34 living in extreme poverty (on less than \$1.90 per day), with the difference anticipated to widen to 121 women for every 100 men by 2030 [<https://www.unwomen.org//media/headquarters/attachments/sections/library/publications/2020/gender-equality-in-the-wake-of-covid-19-en.pdf?1a=en&vs=5142>].

COVID-19 and its Impact

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is the root cause of the ongoing COVID -19 pandemic. In 2019, the SARS-CoV-2 virus, which is closely related to the SARS-CoV virus, caused an outbreak of Novel coronavirus disease. Since its first instance was discovered in December 2019 in Wuhan, China, COVID-19 has rapidly spread over the world, claiming 1,692,230 deaths as of December 20, 2020 [7]. Between 31st December 2019 to 20th December 2020, 76,738,133 cases have been reported so far. The history of coronavirus dates back to 1965 when it was first identified by scientists in humans which led to the common cold. The term “Coronavirus” has been derived from the Latin word Corona which translates to “crown” in English owing to its structural morphology. A novel severe acute respiratory syndrome (SARS) was reported from Southern China in 2002 and 2003, and it spread to around 29 nations. A total

of 8098 people were affected, with 774 deaths reported [8]. The COVID-19 pandemic has wreaked havoc on the population, causing acute health concerns mostly related to respiratory disorders, which include symptoms such as dry cough, fever, sore throat, and loss of taste and smell. Since the outset of the COVID-19 pandemic, the number of new confirmed cases and deaths has been growing continuously, with a global fatality rate of 2.20% and a recovery rate of 70.19% [7]. The current global statistics of the COVID-19 as of 23rd January 2022 are represented in Table 1. India stands second in the list of the most number of confirmed cases with a mortality rate of 1.45%. The worst-hit Indian states have been summarized in Table 2.

Table 1. COVID-effect in ten worst-hit countries as of 23rd January 2022 (<https://www.worldometers.info/coronavirus/countries-where-coronavirus-has-spread/>).

Country	Population	Total Tests	Total Cases	Total Recovered	Total Deaths
USA	334024770	879598015	71,728,557	43892277	489,422
India	1401124519	715520580	39,237,264	35807029	622,979
Brazil	214911839	63776166	23,960,207	21848301	128,514
France	65498431	222105082	16,390,818	9612731	153,787
UK	68441263	440125448	15,784,488	11738323	326,112
Russia	146031913	247600000	11,108,191	9925855	85,784
Turkey	85751692	127511700	10,881,626	9899648	143,296
Italy	60323364	162273201	9,781,191	6450596	91,741
Spain	46782980	66213858	8,975,458	5390818	117,323
Germany	84201113	89622218	8,641,865	7139800	119,103

Table 2. Details of Worst COVID-19 Hit Ten States in India (<https://www.covid19india.org/>).

State	Population (In crore)	Total Testings (In crore)	Total Cases	Total Recovered	Total Deaths
Maharashtra	12.2	6.3	6611078	6450585	140216
Kerala	3.5	3.8	4968657	4857181	31681
Karnataka	6.6	5.1	2988333	2941578	38082
Tamil Nadu	7.6	5.1	2702623	2655015	36116
Andhra Pradesh	5.2	3	2066450	2047722	14373
Uttar Pradesh	22.5	8.4	1710158	1687151	22900
West Bengal	9.7	1.9	1592908	1565471	19141
Delhi	2	2.9	1439870	1414431	25091
Odisha	4.4	2.2	1041457	1029147	8386

Vaccination Hesitancy and Adaptation with Particular Emphasis on Women

Tahmeena Khan¹, Alfred J. Lawrence^{2,*}, Amos Nascimento³ and Rohan Srivastava¹

¹ Integral University, Lucknow, India

² Department of Chemistry, Isabella Thoburn College, Lucknow-226007, Uttar Pradesh, India

³ University of Washington, Tacoma/Seattle, USA

Abstract: The novel beta-coronavirus SARS-CoV-2 (COVID-19) emerged in 2019 in Wuhan from bats and later caused inter-human transmission. India is one of the worst-hit countries, where two million casualties have taken place during the second wave of the pandemic. The year 2021 witnessed the more deadly form of the virus. At the same time, there was remarkable progress in vaccine development resulting in the approval of a few vaccines by the governments. The process of COVID-19 vaccination has kickstarted in many countries. The general attitude towards acceptance of the vaccine has been reported in countries like the USA and Jordan. Very few studies have reported the understanding and hesitation regarding the vaccination among the Indian population, and the present study is an attempt to highlight the general mindset, acceptance, misconceptions and awareness regarding the COVID-19 vaccination from the Indian perspective. Being one of the worst-hit countries in terms of COVID-19, it is important to identify the barriers holding the Indian population back from getting vaccinated. This study was done as a questionnaire survey aimed at knowing the general apprehension, and thoughts of the public regarding the vaccination with 308 respondents, precisely of Indian origin. 58.8% (n=181) respondents were non-vaccinated. 45.2% (n=95) respondents reported that their respective employers made vaccination compulsory. 51.5% (n=120) felt that the vaccine is 60-80% safe. The results may be used by the public health authorities to identify the priority group and the barriers holding people back from vaccination.

Keywords: Acceptance, Concerns, COVID-19, Hesitation, Immunity, India, Longevity, Misconception, Side Effects, Vaccination.

* Corresponding author Alfred J. Lawrence: Department of Chemistry, Isabella Thoburn College, Lucknow-226007, Uttar Pradesh, India: E-mail: Alfred_lawrence@yahoo.com

INTRODUCTION

The coronavirus was first identified in 1965 in studies developed by Tyrrell and Bynoe, who identified a virus that they named B814 [1]. Since then, a morphological similarity was noticed between transmissible cases of ovine bronchitis, hepatitis in rodents and swine gastroenteritis virus. Due to the fact that, morphologically, this type of virus had external projections in the form of a crown, this new group was named “corona virus.” After decades of research, evidence showed that the coronavirus was responsible for respiratory diseases in several animal species, including rodents, sheep, cattle and swine, as well as cats and dogs [2]. Over time, it was discovered that respiratory diseases in humans, especially children.

These correlations remained somewhat unnoticed by the larger public until 2003, when the coronavirus was identified as the cause of a new disease, Severe Acute Respiratory Syndrome (SARS), that emerged in southern China and spread throughout the world quickly. Infectious cases emerged in 29 countries in Asia, the Americas, and Europe, reaching about 8,000 cases and almost 800 deaths. This was followed by several other virological discoveries in Hong Kong (China), Amsterdam (Netherlands), and New Haven (United States) – the latter being called “New Have Coronavirus (HCoV-NH) – as well as international epidemic cases such as the avian flu and swine flu (H1N1) [3]. With technological advances, it was possible to not only carry out serological tests but also to carry out the genetic sequencing of the various types of this virus. In this process, it was concluded that the virus was transmissible not only through the zoonotic route, but also through human vectors. These and other developments in coronavirology led to new hypotheses about the possibility of new epidemics [4].

The novel beta-coronavirus SARS-CoV-2 and the novel coronavirus disease 2019 (COVID-19) emerged in the year 2019 in Wuhan, China, as a result of high-impact zoonoses traced back to bats (order Chiroptera) and viral diseases identified earlier in Southern China [5, 6]. While studies were being carried out to identify its exact origination, COVID-19 reached 188 countries and 25 territories globally, despite the best efforts of governments and the World Health Organization (WHO) [7], due to the high transmission ability of the virus [7]. As the coronavirus is responsible for various respiratory diseases, it spreads by the inhalation of aerosols and through interpersonal contact. While various new vaccines have been developed in different countries, no concrete medicinal cure has been found to date. Therefore, physical distancing, personal hygiene, washing of hands and sanitization with 70% alcohol-based sanitizer have been suggested as precautionary measures to keep the infection at bay [8]. Those suffering from any other co-morbid conditions are at greater risk of getting infected and having

severe symptoms. The incubation period of the virus is said to be of 5.1 days [9]. The symptoms of the disease include fever, dry cough, shortness of breath, chills and dysentery [9].

Coronaviruses are pleomorphic and enveloped with peculiar projections protruding from their surface consisting of S protein. The genome of the novel coronavirus is transcribed in 10 open reading frames (ORFs), translating into a polyprotein processing into 16 non-structural proteins (NSPs) [10]. The non-structural proteins help in genome replication, capping, tailing, which are necessary for the maintenance of the virus [11]. The SARS-CoV-2 virus also contains four structural proteins, namely spike (S), nucleocapsid (N), envelope (E), and membrane (M) proteins encoded by the 3-end of the viral genome [12]. Amongst the four structural proteins, the S glycoprotein, being a multi-functional trans-membrane protein, has an important role in viral attachment and its entry into the host cell [12]. The S protein consists of S1 and S2 subunits splitting into different functional domains. The S1 subunits consist of two domains viz. N-terminal Domain (NTD) and Receptor Binding Domain (RBD), consisting of conserved receptor binding motif (RBM) [13]. Immunotherapy is one of the most efficient methods used for the cure of different contagious diseases and cancer. The technique included the activation of the immune system to enhance the immune response [14]. The COVID-19 vaccines are usually targeted with an aim to generate S protein-neutralizing antibodies. Studies have found almost no cross-neutralization between the sera of SARS-CoV and SARS-CoV-2, showing that those recovering from one infection are not necessarily safe from the other [15]. More than five thousand full-length genomes of SARs-CoV-2 have been derived from different nations, which delineate the polymorphisms in S and other proteins of the virus responsible for vaccine development. Most of the vaccines developed against COVID-19 have been using S-protein [16]. Multiple nations across the globe have initiated vaccination under emergency authorization, and US FDA has approved Pfizer and Moderna, whereas the UK regulatory bodies have approved three vaccines viz., Pfizer, AstraZeneca and Moderna based on the efficacy and safety data obtained from phase III trials. India being one of the worst-hit countries, has approved two vaccines and initiated its largest vaccination drive initially from frontline workers and older adults. Pune-based Serum Institute's Covishield and Hyderabad-based Bharat Biotech's Covaxin have been approved by the Indian government. Covishield has passed the phase III trials, whereas Covaxin is still undergoing phase III trial [17]. The approved vaccines are based on either inactivated or active attenuated viruses, protein-sub units, virus-like particles (VLP), replicating and non-replicating viral vectors, DNA, RNA, and nano-particles, *etc.*, showing their own exclusive properties [18]. To augment the immunogenicity, various adjuvant techniques like AS03 (GSK), MF-59 (Novartis), CpG 1018 (Dynavax), *etc.*, are also available for the effective

Computational Drug Discovery Against COVID-19

Shristi Modanwal¹, Viswajit Mulpuru¹ and Nidhi Mishra^{1,*}

¹ Department of Applied Sciences, Indian Institute of Information Technology Allahabad, Prayagraj, India

Abstract: The global spread of Severe Acute Respiratory Syndrome coronavirus 2 (SARS-CoV-2), which causes the disease COVID-19, has increased drastically since the first cases in Wuhan, People's Republic of China, at the end of 2019. There is no single drug that can be used specifically to treat COVID. The crucial stage in the drug development process is screening huge libraries of bioactive molecules against a biological target, usually a receptor or a protein. Virtual Screening (VS) has become a valuable tool in the drug development process as it allows for efficient *in silico* searches of millions of compounds, resulting in higher yields of possible therapeutic leads, and is cost-effective. The spread of the SARS-CoV-2 virus presents a major threat to world health and has resulted in a global crisis because of the high mortality rate and absence of clinically authorised treatments and vaccines for COVID-19. Finding effective drugs or repurposing available antiviral drugs is a critical need in the fight against COVID-19. VS can be classified as either Structural-Based Virtual Screening or Ligand-Based Virtual Screening. VS techniques have been widely applied in the field of antiviral drug design and have aided in the identification of new compounds as possible anti-viral drugs. Both LBVS and SBVS approaches have proved extremely helpful in identifying several prospective anti-viral drugs with nanomolar range. VS, in contrast to experimental approaches, is quick and cost-effective on the one side but has low prediction accuracy on the other.

Keywords: Ligand-Based Virtual Screening, SARS-CoV-2, Structure-Based Virtual Screening.

INTRODUCTION

Novel drug development is a costly and time-consuming process that can cost billions of dollars and take up to ten years. While most of the money was spent on experimental research to find new drug candidates in the hopes of finding one with biological activity against a target protein a few decades ago, computer-aided drug discovery (CADD) methodologies have garnered interest in recent years because they can reduce the number of ligands that must be tested in experimental

* Corresponding author Nidhi Mishra: Indian Institute of Information Technology, Prayagraj, India; E-mail: nidhimishra@iitaa.ac.in

assays. One of the most essential and extensively used CADD techniques in virtual screening (VS) [1]. VS is an *in-silico* approach for estimating the activity of active molecules/ compounds to identify them. Due to its ability to minimize the cost of screening while also increasing the hit rate, it has become a popular complementary and alternative method to experimental high-throughput screening technologies for drug discovery and development in recent years [2]. Virtual screening uses a large library of small compounds to perform a docking algorithm/calculation to find the conformation and molecular orientation that produces the best score between each small molecule and a target protein. The results are then sorted to provide a list of compounds that are anticipated to bind to a protein target with decreasing strength. To find and validate new drug leads, these predictions can be put to the test in the lab [3]. It also aids in the testing of currently available small compounds for other different diseases. In the field of drug development, VS is one of the most reliable and accurate methods.

A deadly and highly infectious viral disease has recently emerged in Wuhan, China, with the causative agent being identified as a new coronavirus, called Coronavirus disease 2019 (COVID-19) [4, 5]. Resultant of the pandemic of COVID-19, several researchers used a virtual screening approach for drug design and repurposing of pre-existing pharmaceuticals and natural products. The epidemic was so severe that the World Health Organization (WHO) was constrained to designate it as a pandemic just a month after it began to spread widely [6]. The SARS-CoV-2 virus belongs to the order Nidovirales and the family Coronaviridae with a single-stranded positive-sense RNA genome enclosed within a membrane envelope. SARS-CoV-2 is a member of the β coronavirus genus, which also includes the SARS coronavirus (SARS-CoV) and the Middle East respiratory syndrome coronavirus (MERS-CoV) (MERS-CoV) [7]. There are seven types of coronavirus that have been identified as infecting humans (COVID-19) and these are severe acute respiratory syndrome coronavirus (SARS-CoV), Human Coronavirus 229E (HCoV-229E), Human Coronavirus NL63 (HCoV-NL63), Middle East respiratory syndrome coronavirus (MERS-CoV), Human Coronavirus OC43 (HCoV-OC43), Coronavirus Disease 2019 (COVID-19), and Human Coronavirus HKU1 (HCoV-HKU1). Among these, SARS-CoV and MERS-CoV viruses are highly transmissible and pathogenic infections in humans [8]. Coronaviruses cause respiratory, neurological, gastrointestinal systems, and hepatic disorders, as well as serious and sometimes fatal infections. Human-to-human aerosol transmission, which occurs mostly through contaminated droplets, hands, or surfaces, is without a doubt the most common cause of infection. SARS-CoV-2 (novel coronavirus) spreads mostly through the respiratory system and uses Angiotensin-Converting Enzyme 2 (ACE2) receptor, which is the same as SARS-CoV [9].

Consequently, the number of affected people continues to rise, and no effective treatments have yet been discovered. As a result, the need for medications to treat COVID-19 is critical. The coronavirus has the most significant structural proteins, namely Spike Proteins(S), Membrane Proteins (M), Nucleocapsid Proteins (N), and Envelope Proteins (E) [10]. These proteins are required for viral genome replication, synthesis, virion, and viroporin formation, virion-receptor attachment, which all contribute to the virus's ability to enter and multiply in a host organism, spreading infection [11]. In addition to mentioned structural proteins, replicase proteins, Main protease or Chymotrypsin-like protease (Mpro or 3CLpro), and papain-like protease (PLPRO) play an important role in the pathogenesis of SARS-CoV-2 [12]. Proteins such as Rna-directed RNA polymerase (RdRp) and Non-structural protein 15 (nsp15), nsp 16 can also be used as targets. SARS HCoV has the RdRp that is most similar to SARS-CoV-2, so the SARS-CoV-2RdRp model should be built as a homolog of the SARS HCoV RdRp [13].

VIRTUAL SCREENING METHODS

Virtual screening is currently a standard procedure in drug discovery before wet-lab studies. When several drug candidates, and other drug-like small molecules bind to a specific protein, Virtual Screening is used to short-list significant candidates by estimating the estimated affinities and possible binding mechanisms of these compounds. Even while VS is far less expensive than lab research, it still necessitates the installation of appropriate High-Performance Computing infrastructure to screen huge ligand libraries [14]. The availability of high-resolution structures of many of the SARS-CoV-2 proteins aided us in quickly identifying lead therapeutic candidates for SARS-CoV-2 using *in silico* screening methods. Virtual Screening can be Structural Based Virtual Screening (SBVS) and Ligand Based Virtual Screening (LBVS). Based on structural activity data from a pool of known active compounds, LBVS identifies promising compounds for laboratory experiments. The LBVS method includes quantitative structure-activity relationship (QSAR), pharmacophore mapping, similarity and substructure searches, and 3D shape matching. SBVS, on the other hand, docks potential molecules and ranks them according to their expected binding affinity to the binding site utilizing the biological target's 3D structure, which was either determined experimentally through X-ray crystallography or NMR or computationally through homology modeling [15, 16]. SBVS is the best approach for discovering novel ligands when the target protein's 3D structure has been experimentally determined. When the target's 3D structure is unknown or prediction using structure-based approaches is problematic, LBVS is the best procedure [1]. A schematic representation of Virtual Screening and its categories is shown in (Fig. 1).

CHAPTER 7

Methods in Drug Repurposing: Emphasis on COVID-19

Akhilesh Kumar Maurya¹ and Nidhi Mishra^{1,*}

¹ Chemistry Laboratory, Department of Applied Sciences, Indian Institute of Information Technology Allahabad, Prayagraj, 211012, India

Abstract: Coronavirus disease 19 (COVID-19) is a pandemic situation caused by the SARS-CoV-2 (severe acute respiratory syndrome coronavirus 2), and dedicated medical research finding to cure the disease are rapidly evolving globally. SARS-CoV-2 is a highly mutating virus having various strains, till the reporting of this study, COVID-19 has 5 variants, *i.e.*, Alfa, beta, gamma, delta, and omicron. A potential way for drug development is drug repurposing has got a lot of attention. Drug repurposing is the easiest and safest way to find out the drugs to cure COVID-19. Various new drugs have been discovered and are under clinical trial for the treatment of disease. Combinatorial treatments of COVID-19 patients give a very positive response in the treatment of SARS-CoV-2. The various vaccine already has been developed to produce antibodies against COVID-19. However, a large number of research studies have been done on COVID-19. This study is dedicated to research on COVID-19 therapy by the repurposing of existing drugs and methods used for the drug repurposing.

Keywords: Combinatorial, COVID-19, Drug Repurposing, Medical Research, SARS-CoV-2, Targeted Based Approaches.

INTRODUCTION

The pandemic potential of new or mutated viruses has been increasing over the past few decades, as evidenced by epidemic and pandemic storms of the Middle East respiratory virus (MERS-CoV), Human Immunodeficiency Virus (HIV), Ebola virus (EBOV), Zika virus (ZIKV), for which we have still no drugs or lack of specific therapy [1]. World Health Organization (WHO) endeavour to be “the global guardian of health” are repeatedly conquered by the arrival of COVID-19 disease caused by the coronavirus. With over 2.4 Billion confirmed COVID-19 cases and 4.8 million people death recorded worldwide [2] and counting continues, the pandemic outbreak of COVID-19 was declared by WHO on March 11, 2020 [3]. Albeit huge advancements have been made to comprehend

* Corresponding author Nidhi Mishra: Chemistry Laboratory, Department of Applied Sciences, Indian Institute of Information Technology Allahabad, Prayagraj, 211012, India; E-mail: nidhimishra@iiita.ac.in

and cure Coronavirus, the flow pandemic has, generally, overpowered drug organizations to facilitate the improvement of antibodies and medications against this clever sickness. The lethargic speed in clever medication advancement, combined with high steady loss rates and expanding administrative obstacles, has provoked medication engineers to consider another medication improvement technique: drug repurposing.

The COVID-19 virus is a capsulated RNA (ribonucleic acid) virus, from the genus β -coronavirus, *i.e.*, present in bats, aves, and other mammals, including humans [4]. Coronavirus have four subfamilies: δ (delta), Υ (gamma), β (beta), and α (alpha) coronaviruses. Among these, α and β -coronavirus come from mammals, especially from bats; Υ and δ - variant of coronaviruses arise from pigs and aves [5]. Coronavirus has a genome of single-stranded RNA (ssRNA) that is confined with a capsulated structure of proteins [6].

Designing and developing new therapeutic drugs with an exhaustive profile of the COVID-19 virus is a time-taking, costly, and challenging process. To reduce these, drug repurposing (also known as repositioning or rediscovery) is an interesting way to accelerate the recognition of drugs from the existing databases of drugs that can cure or treat COVID-19 [7]. Drug repurposing or repositioning may help us to find new therapeutics for any diseases in a short time with low costs, basically when the clinical and or preclinical and trials and safety test experiments have been completed for drug molecules [8]. The basic motto of drug repositioning is to hike the curative use of previously usable medicine for more and new medical treatment purposes [9]. Computational approaches for repurposing drugs attempt new testable expectations for the standardized reuse of available tested drugs [10].

Drug Repurposing Methods

Like every drug repurposing project, Drugs repurposing under COVID-19 follow these three steps [11]:

1. Identifying the candidate drug;
2. Mechanistic evaluation of the preclinical models of effect drug; and
3. Assessment of the drug candidature.

The systematic approach to the re-use of medicines is widely divided into *in silico*/ computational and experimental methods. However, it should be recognized that these methods can be utilized in synergy to obtain the foremost reassignment result.

Computational Methods

Structure-Based

Possibly one of the most common approaches to reallocating medications in the pandemic of SARS-CoV-2 disease. Structure-based screening analyses for SARS-CoV-2 inhibitors have been highly recorded in numerous research studies worldwide, due to the high computing capacity and availability of three-dimensional structures of drug molecules and receptor target proteins and nucleic acid [12]. Structure-based screening of ligands or drug molecules is an *in silico* method used in the initial phase of a medication repurposing drive to look for biologically active compounds against certain therapeutic targets, based on receptor binding site complementarity in a compound library. This computational virtual screening can be done in two steps [13].

1. Molecular docking is carried out on many previously available drugs or drug library applicants to link the 3-D structure of a target receptor obtained by NMR, X-ray approaches, or computational modelling methods.
2. A score of binding affinity is used to compute the probability of all drugs/ligands connecting the target molecule with high affinity, giving antique repurposing hits.

Because of knowledge of its antecedents (SARS-CoV-2 and MERS-CoV), the cellular targets are very well defined. This target-centric strategy is particularly useful, potentially eliminating the necessity to illuminate the action mode of hits. As a result, several medications may be tested against a specific target receptor (such as Angiotensin-Converting Enzyme-2 (ACE2), Main Protease), as in the normal docking method. Elfiky used ordinary sub-molecular docking techniques, including coronavirus RNA-dependent RNA polymerase (RdRP), to evaluate for expected drug molecules such as SARS-CoV-2 inhibitors, virtual screening presently supported inhibitors of polymerase medications and discovered remdesivir, ribavirin, galidesivir, and tenofovir is a powerful suppressor of RdRP enzymes, with restricting the value of energies between -7.0 to -7.8 kcal/mol [14].

Toremifene is an example of a viral inhibitor drug based on target repurposing. Martin and Cheng initially found toremifene as a possible COVID-19 drug molecule, followed by docking methodology up to spot the toremifene target molecules. They are successful with known 2 effective targets, particularly the spike-conjugated protein and NSP14 [15].

CHAPTER 8

Virtual Screening of Phytochemicals in Search of a Potential Drug Candidate for COVID-19: DFT Study and Molecular Docking

Nikita Tiwari^{1*}, Lubna Jamal¹ and Anil Mishra¹

¹ Department of Chemistry, University of Lucknow, Lucknow-226007, Uttar Pradesh, India

Abstract: The global health pandemic due to COVID-19 caused by SARS-CoV-2, affected and changed the world's condition drastically. Herein, we evaluated the bioactivity of some phytochemicals as inhibitors against SARS-CoV-2 M provirus (6LU7) using computational models. We reported the optimization of phytochemicals employing density functional theory (DFT) with B3LYP/6-311G+(d,p) level theory. DFT calculations were employed to determine the free energy, dipole moment as well as chemical reactivity descriptors. Molecular docking has been performed against the SARS-CoV-2 M provirus to search the binding affinity and interactions of all compounds with the respective protein. The known drug, Chloroquine of SARS-CoV-2 main protease, was also docked to evaluate its binding affinity. Besides, the data from DFT, the docking studies predicted that flavonoids (Quercetin, Myricetin, Apigenin and Daidzein) have the least binding affinity and might serve as a potent inhibitor against SARS-CoV-2 comparable with the approved medicine, Chloroquine. The high binding affinity of flavonoids was attributed to the presence of hydrogen bonds along with different hydrophobic interactions between the flavonoid and the critical amino acid residues of the receptor. The DFT calculations showed that flavonoids have high-lying HOMO, electrophilicity index and dipole moment. All these parameters could share a different extent to significantly affect the binding affinity of these phytochemicals with active protein sites.

Keywords: Apigenin, B3LYP, Chloroquine, COVID-19, DFT Calculations, Daidzein, Dipole Moment, Electrophilicity Index, Flavonoids, HOMO, Hydrogen Bonds, Hydrophobic Interactions, Molecular Docking, Myricetin, Pandemic, Phytochemicals, Quercetin, SARS-CoV-2.

INTRODUCTION

In the final month of the year 2019, a major cluster of strange pneumonia due to a novel coronavirus was reported in Wuhan metropolis, China [1]. Despite efforts to

* Corresponding author **Nikita Tiwari:** Department of chemistry, Lucknow University, Lucknow-226007, Uttar Pradesh, India: E-mail: nikitalko23@gmail.com

include the outbreak inside the preliminary place, the dissemination of SARS-CoV-2 has continued to spread widely to different countries. Therefore, in March 2020, the WHO declared the uncontrollable spread of SARS-CoV-2 as a pandemic [2]. Now, after more than two years after the initiation of the infection, this disease is still a threat to human life [3]. The control of SARS-CoV-2 is the need of the hour not only for human health but also for the prosperity of the nations and the betterment of society, and to achieve this purpose, global collaborations are very important [4].

Coronavirus (CoV), the virus responsible for COVID-19, belongs to the family Coronaviridae. They have spikes on their surfaces and contribute to a huge group of viruses containing RNA genome [5]. Based on the genetic and serological relationship, the coronaviruses are broadly classified into four major groups-Alpha, Beta, Gamma and Delta [6]. These RNA viruses are mainly distributed among birds and mammals [7] and have a very high potential to infect the human respiratory system [7, 8]. HCoV-OC43, -229E, -NL63, -HKU1, SARS-CoV (Severe Acute Respiratory Syndrome – Coronavirus), MERS-CoV (Middle East Respiratory Syndrome – Coronavirus) and now SARS-CoV-2 are a few examples of coronaviruses that infect humans [6, 9].



In the search for the cure, complete knowledge of the cause is pretty much important. Cryogenic electron microscopic studies and many other studies show that SARS-CoV-2 binds to the cell membrane of ACE2 (Angiotensin-converting enzyme 2) [10, 11]. The genome of coronavirus carries two replicase polyproteins that undergo proteolytic processing into a set of mature NSP (non-structural proteins) that function during viral replication, including RdRp, 3CL-Mpro, Papain-like proteinase (PL2pro) and a superfamily 1-like helicase (HEL1) [12]. According to the structure, the genome of SARS-CoV-2 (novel coronavirus) encodes many important proteins for its replication in the host genome, such as M (membrane protein), S (spike protein), N (nucleocapsid protein), E (envelop protein) and coronavirus main protease. These proteins play a pivotal role in gene expression and cleave polyproteins into replication-related proteins [13, 14]. The structure of 3CL-Mpro comprises three domains, *i.e.*, I, II and III, where domains I and II are N-terminal domains while domain III is a C-terminal domain [15].

To control and cure the SARS-CoV-2 infection, drug designing and development of the vaccine are necessary. Nowadays, many researchers around the globe are involved in studying chemicals with anti-viral properties. Many naturally occurring phytochemicals have anti-viral effects and pharmacological properties [16]. According to the ancient Indian texts ‘SUSHRUT SAMHITA’ and ‘CHARAK SAMHITA’ ancient people used the different parts of plants to cure themselves of various infectious diseases [17, 18]. *Toona sinensis* [18, 19],

Jatropha curcas [18, 20], *Glycyrrhiza glabra* [18, 21], *Daucus carota* [18, 22], *Piper chaba* [18, 23], *Cinnamomum zeylanicum* [18, 24], *Zingiber officinale* [18, 25], etc. are some common plants that are used to treat the diseases since ancient times, or we can say that their therapeutic uses are well known. Different parts of these plants contain a large number of phytochemicals (Table 1), and the medicinal properties of these phytochemicals provide them with a very special place in the field of drug design or medicinal research. So we can say that phytochemicals may provide potential solutions to the SARS-CoV-2 pandemic.

The inhibition property of phytochemicals is related to their ability to inhibit the virus from attaching to the 3CL-Mpro [29, 30]. In this work, we studied certain phytochemicals (*apigenin, benzoic acid, daidzein, furfural, furfuryl formate, gallic acid, 4-hydroxybenzoic acid, maltol, oxalic acid, pyragallol, salicylic acid, succinic acid, 2,3-butanediol, propionic acid, eugenol, cinnamaldehyde, caffeic acid, pentanol, piperonal, 2,3,5-trimethyl pyrazine, asparagine, quercetin, mercytin*) to understand their utility in drug designing and effectiveness against SARS-CoV-2 via DFT calculations and molecular docking. Molecular docking is a robust, effective, low-cost and less time-consuming process than traditional drug discovery methods [31]. *Chloroquine* is taken as a reference compound for this study.

Table 1. Plants and their constituent chemicals active against virus diseases.

Plants	Plant Image	Family	Part Used	Chemicals
<i>Jatropha curcas</i>	 [26]	Euphorbiaceae	Leaves, Latex	Apigenin, benzoic acid, daidzein, pyragallol, salicylic acid, gallic acid
<i>Glycyrrhiza glabra</i>	 [27]	Leguminosae	Root	Pentanol, furfural, Furfuryl formate, maltol, butanediol, propionic acid

Role of Immunity Against COVID-19

Nidhi Singh^{1,*}

¹ Department of Chemistry, Isabella Thoburn College, Lucknow-226007, India;

Abstract: The chapter defines the importance of immunity against COVID-19. The chapter describes the immunopathogenesis of COVID-19 and the way the body fights back and shows its immune response against the pathogen. Factors affecting immunity include ageing and obesity. The effect of the age factor has been visible in the suffering due to the coronavirus. The chapter also describes the nutritional factors that could boost immunity and enhance the immune response of the body against COVID-19. The major nutritional elements comprise vitamins and micronutrients, responsible for the biosynthesis of amino acids and strengthening of the defence system of the body. Natural products also play an important role in the enhancement of immunity against the coronavirus. The phytoconstituents present in plants play an active biochemical role in controlling COVID-19 symptoms. Vaccination has also helped in gaining acquired immunity against the COVID-19 pathogen and helped in developing herd immunity as well.

KEYWORDS: COVID-19, Immunity, Immunopathogenesis, Herd Immunity, Micronutrients, Phytoconstituents, Vaccination, Vitamins.

INTRODUCTION

Immunity is the natural defence system of human beings to protect them against various pathogenic diseases. Certain barriers evolved cell types, and antigen-antibody response relationships form the basis of human immunity. It is a response that is always active and is enhanced in times of infection. The importance of immunity is highly marked in our lives. A most recent example of this is being witnessed, as the world is in the clutches of coronavirus or COVID-19. The virus was named such, because of its initiation in the year 2019. It has been two years since then, and the virus continues to create havoc in the world. Various studies and reports have shown the importance or role of immunity during this pandemic [1, 2]. People with higher immunity have better survived this pandemic, rather than the ones with compromised immunity. It can be

* Corresponding author Nidhi Singh: Department of Chemistry, Isabella Thoburn College, Lucknow,-226007, India; E-mail: nidhi.singh23081993@gmail.com

witnessed through the case of children, who were least affected by this virus, as they had stronger immunity than elderly people. Since coronavirus came as a new virus variant and elderly people had no memorized or acquired immunity against it, they suffered the most as most of them had other comorbidities like diabetes, blood pressure, heart problems, or respiratory problems. Coronavirus effect combined with these morbidities proved fatal to many of them. The spread of the virus was also rapid, as there was no underlying immunity against this virus. Thus, it can be deduced that immunity plays an important role against the COVID-19 virus [3, 4].

Coronavirus causes an outbreak of severe acute respiratory disorder wherein the virus disrupts the functioning of respiration, causing heavy breathing and loss of breath. In acute cases, the patient needs to be shifted to a ventilator as the virus may gradually attack other organs as well, and the patient may die of multiple organ failure.

Immune System: Process and Defense

The immune system consists of natural and acquired immunity. Innate or natural immunity exists from birth, like barriers or first-line defence, while acquired immunity refers to immunity acquired over the years based on memorization of their antigen-antibody responses to pathogens [5]. The general functions of the immune system for effective defence include:

1. Creation of barriers for the prevention of pathogens.
2. Identification of pathogens after their entry.
3. Elimination of pathogens.
4. Generation of immunological memory.
5. (Fig. 1) depicts the immune system process and defense mechanism by means of a flowchart.

Creation of Barriers for the Prevention of Pathogens

The natural or first-line defence of our immune system are the natural barriers, which prevent the entry of pathogens from external environment, into our body. These natural barriers include physical barriers, chemical barriers, or biological barriers. Physical barriers include skin, mucosal layer of gastrointestinal tract, mucosal layer of genitourinary tract and mucosal layer of respiratory tract. Chemical barriers include the acidic pH of stomach, which destroys the pathogen before reaching its target site through the bloodstream. Besides this, sweat, saliva, mucus and tears also act as chemical barriers in the immune system, as they contain lysozyme, which destroys the pathogen, thereby preventing its entry into

our body. Biological barriers to the immune system include common organisms on the skin and gut, which are harmless and use up food and space so that pathogenic bacteria do not have a chance to colonize themselves. Other than this, secretions like IgA (immunoglobulins) also act as an important biological barrier to immunity [6].

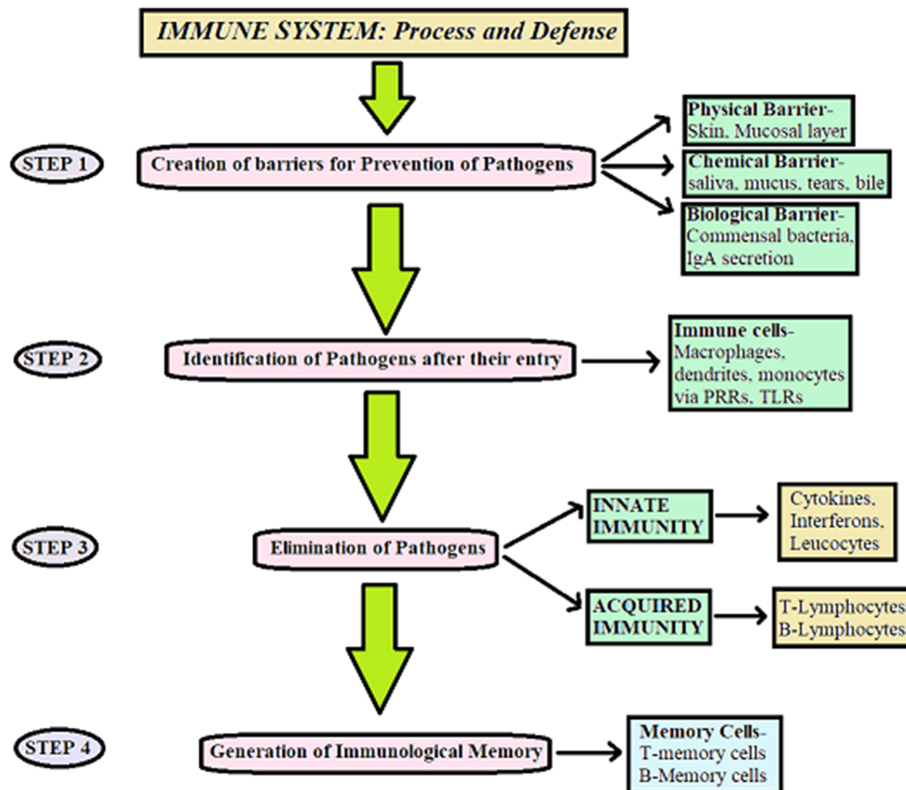


Fig. (1). Flowchart representing Immune system process and defense mechanism.

Identification of Pathogens After their Entry

Immune cells like macrophages, dendrites and monocytes of the innate immunity system are responsible for the recognition or identification of pathogens upon their entry. The recognition process depends upon pattern recognition receptors (PRRs), present on the immune cell’s surface, which identify the molecular structure of the pathogen. This molecular structure is broadly similar to most kinds of pathogens and is termed microbe-associated molecular patterns (MAMPs) or pathogen-associated molecular patterns (PAMPs). The pattern recognition receptors consist of different toll-like receptors (TLRs), each of which is responsible for the identification of different pathogens like bacteria, viruses, fungi, and other parasites. Viruses are particularly identified by intracellular

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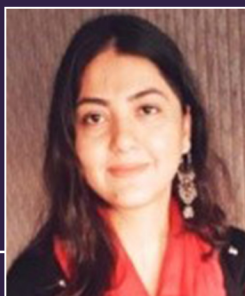
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Tahmeena Khan

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.