

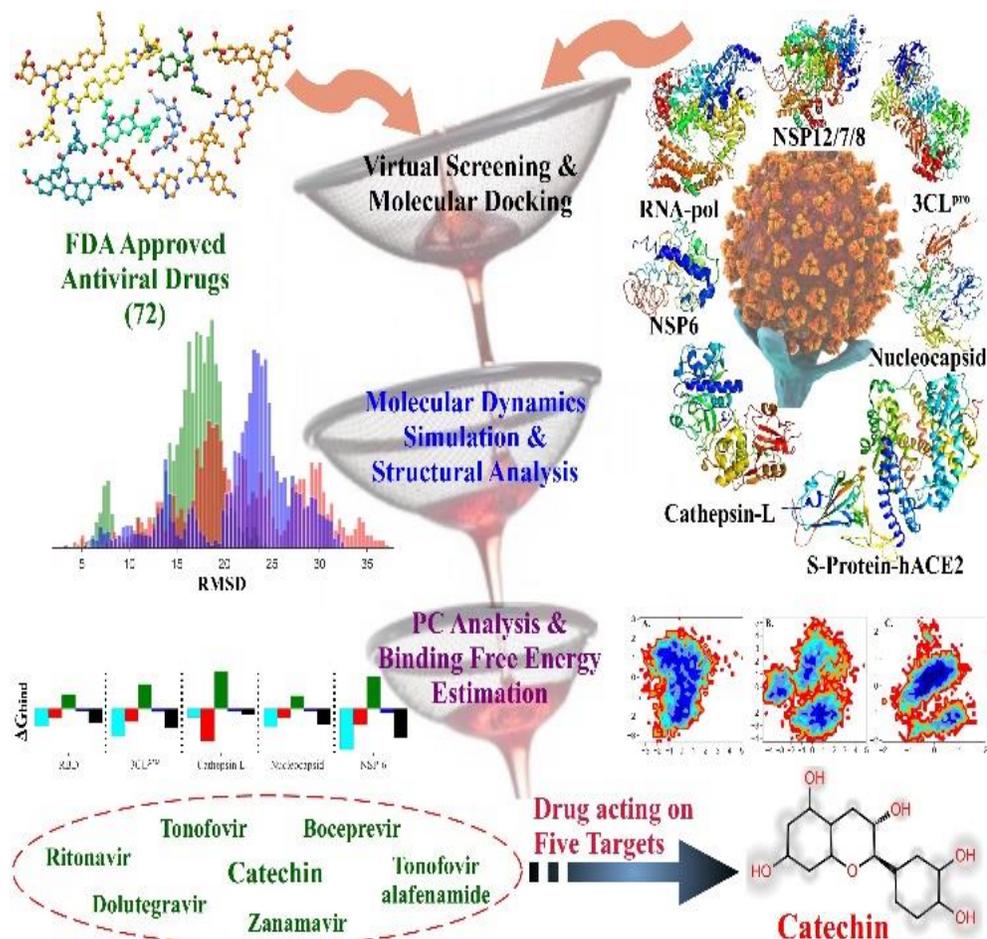
Research Grants at AUH during COVID-19

Project title	Funding agency	Amount	Principal Investigator
Development of onspot diagnostic kit for COVID19 based on RT-LAMP Integrated CRISPR-Cas technique	BRNS	16.56 Lakhs	Dr. Saif Hameed, AIB, AUH
A low cost portable microfluidics embedded on chip RT-PCR and microelectrode array coupled point-of care optoelectronic device for large scale screening of emerging viral disease like SARS COV2	DBT- BIRAC	90.00 Lakhs	Dr. Ranjita Ghosh Moulick, AIB, AUH
3D Manufacturing of N95 Mask having Inherent Antimicrobial Properties	IDE 2.0 MleTY G3C	4.5 Lakhs	Dr Atul Thakur, AINT, AUH
An Antimicrobial Face-Mask Using Nano-particle Coating	IDE 2.0 MleTY G3C	4.5 Lakhs	Dr. Arvind Chhabara ASCI, AUH



Identifying the Natural Polyphenol Catechin as a Multitargeted Agent Against SARS-CoV-2 For the Plausible Therapy of COVID-19: An integrated Computational Approach

Chandra Bhushan Mishra^{1†}, Preeti Pandey^{2†}, **Ravi Datta Sharma**^{3†}, Md. Zubair Malik⁴, Raj Kumar Mongre¹, Andrew. M. Lynn⁴, **Rajendra Prasad**^{3,5}, Raok Jeon^{1*} and **Amresh Prakash**^{5*}



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Case Study

Identifying the natural polyphenol catechin as a multi-targeted agent against SARS-CoV-2 for the plausible therapy of COVID-19: an integrated computational approach

Chandra Bhushan Mishra[†], Preeti Pandey[†], Ravi Datta Sharma[†], Md. Zubair Malik, Raj Kumar Mongre, Andrew M. Lynn, Rajendra Prasad, Raok Jeon and Amresh Prakash

Corresponding authors: Amresh Prakash, Amity Institute of Integrative Sciences and Health (AIISH), Amity University Haryana, Gurgaon 122413, India. E-mail: amreshprakash@jnu.ac.in, aprakash@ggn.amity.edu; Raok Jeon, College of Pharmacy, Sookmyung Women's University, Cheongpa-ro 47-gil 100, Yongsan-gu, Seoul, 04310, Republic of Korea. E-mail: rjeon@sookmyung.ac.kr
[†]These authors contributed equally to this work.

Abstract

The global pandemic crisis, coronavirus disease 2019 (COVID-19), caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has claimed the lives of millions of people across the world. Development and testing of anti-SARS-CoV-2 drugs or vaccines have not turned to be realistic within the timeframe needed to combat this pandemic. Here, we report a comprehensive computational approach to identify the multi-targeted drug molecules against the



Pandey P, Rane JS, Chatterjee A, Kumar A, Khan R, **Prakash A***, Ray S*. Targeting SARS-CoV-2 spike protein of COVID-19 with naturally occurring phytochemicals: an *in-silico* study for drug development. **J Biomol Struct Dyn.** 2020 Jul 22:1-11. doi: 10.1080/07391102.2020.1796811.

Targeting SARS-CoV-2 spike protein of COVID-19 with naturally occurring phytochemicals: an *in silico* study for drug development

Preeti Pandey^{a#}, Jitendra Subhash Rane^{b#}, Aroni Chatterjee^{c#}, Abhijeet Kumar^{d#}, Rajni Khan^e, Amresh Prakash^f and Shashikant Ray^g

^aDepartment of Chemistry & Biochemistry, University of Oklahoma, OK, USA; ^bDepartment of Biosciences & Bioengineering, Indian Institute of Technology Bombay, Mumbai, India; ^cIndian Council of Medical Research (ICMR)—Virus Research Laboratory, NICED, Kolkata, India; ^dDepartment of Chemistry, Mahatma Gandhi Central University, Motihari, India; ^eMotihari College of Engineering, Motihari, India; ^fAmity Institute of Integrative Sciences and Health, Amity University Haryana, Gurgaon, India; ^gDepartment of Biotechnology, Mahatma Gandhi Central University, Motihari, India

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ABSTRACT: Spike glycoprotein, a class I fusion protein harboring the surface of SARS-CoV-2 (SARS-CoV-2S), plays a seminal role in the viral infection starting from recognition of the host cell surface receptor, attachment to the fusion of the viral envelope with the host cells. Spike glycoprotein engages host Angiotensin-converting enzyme 2 (ACE2) receptors for entry into host cells, where the receptor recognition and attachment of spike glycoprotein to the ACE2 receptors is a prerequisite step and key determinant of the host cell and tissue tropism. Binding of spike glycoprotein to the ACE2 receptor triggers a cascade of structural transitions, including transition from a metastable pre-fusion to a postfusion form, thereby allowing membrane fusion and internalization of the virus. From ancient times people have relied on naturally occurring substances like phytochemicals to fight against diseases and infection. Among these phytochemicals, flavonoids and non-flavonoids have been the active sources of different anti-microbial agents. We performed molecular docking studies using 10 potential naturally occurring compounds (flavonoids/non-flavonoids) against the SARS-CoV-2 spike protein and compared their affinity with an FDA approved repurposed drug hydroxychloroquine (HCQ). Further, our molecular dynamics (MD) simulation and energy landscape studies with fisetin, quercetin, and kamferol revealed that these molecules bind with the hACE2-S complex with low binding free energy. The study provided an indication that these molecules might have the potential to perturb the binding of hACE2-S complex. In addition, ADME analysis also suggested that these molecules consist of drug-likeness property, which may be further explored as anti-SARS-CoV-2 agents.

ABSTRACT

Spike glycoprotein, a class I fusion protein harboring the surface of SARS-CoV-2 (SARS-CoV-2S), plays a seminal role in the viral infection starting from recognition of the host cell surface receptor, attachment to the fusion of the viral envelope with the host cells. Spike glycoprotein engages host Angiotensin-converting enzyme 2 (ACE2) receptors for entry into host cells, where the receptor recognition and attachment of spike glycoprotein to the ACE2 receptors is a prerequisite step and key determinant of the host cell and tissue tropism. Binding of spike glycoprotein to the ACE2 receptor triggers a cascade of structural transitions, including transition from a metastable pre-fusion to a post-fusion form, thereby allowing membrane fusion and internalization of the virus. From ancient times people have relied on naturally occurring substances like phytochemicals to fight against diseases and infection. Among these phytochemicals, flavonoids and non-flavonoids have been the active sources of different anti-microbial agents. We performed molecular docking studies using 10 potential naturally occurring compounds (flavonoids/non-flavonoids) against the SARS-CoV-2 spike protein and compared their affinity with an FDA approved repurposed drug hydroxychloroquine (HCQ). Further, our molecular dynamics (MD) simulation and energy landscape studies with fisetin, quercetin, and kamferol revealed that these molecules bind with the hACE2-S complex with low binding free energy. The study provided an indication that these molecules might have the potential to perturb the binding of hACE2-S complex. In addition, ADME analysis also suggested that these molecules consist of drug-likeness property, which may be further explored as anti-SARS-CoV-2 agents.

Abbreviations: COVID-19: Coronavirus Disease 2019; SARS-CoV-2S: Severe Acute Respiratory Syndrome Coronavirus 2 Spike Protein; hACE2: Human Angiotensin Converting Enzyme-2; hACE2-S protein complex: Human Angiotensin Converting Enzyme-2 receptor and Severe Acute Respiratory Syndrome Coronavirus 2 Spike protein complex; HCQ: Hydroxychloroquine; CQ: Chloroquine; ACE2: Angiotensin-Converting Enzyme-2; MERS-CoV: Middle East Respiratory Syndrome coronavirus; PDB: protein data bank; ADME: absorption, distribution, metabolism and excretion

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KEYWORDS

COVID-19; molecular docking; phytochemicals; flavonoids and non-flavonoids

1. Introduction

The world population is facing a severe mass annihilation due to the rise of a global pandemic named Coronavirus Disease 2019 (COVID-19) (Boopathi et al., 2020; Chatterjee et al., 2020; Joshi et al., 2020; Kirchdoerfer et al., 2016). This pandemic is caused by a novel single-stranded RNA virus belonging to the β -coronavirus genera of the coronaviridae family (Elfiky & Azzam, 2020; Enmozhi et al., 2020; Khan et al., 2020; Rajarshi, Chatterjee & Ray 2020; Sarma et al., 2020; Sinha et al., 2020). As this virus shares significant

phylogenetic similarity and structural familiarity (about 80% nucleotide identity and 89.10% nucleotide similarity) with the severe acute respiratory syndrome coronavirus (SARS-CoV), it has been named as Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) and placed in the same lineage (Subgenus *Sarbecovirus*) (2020; Boopathi et al., 2020; Das et al., 2020; Khan et al., 2020; Ou et al., 2020; Rajarshi, Chatterjee & Ray 2020). To date, no effective regime of antivirals or vaccines is available for the use of the general public to combat the effect of COVID infections, which has put the population at a more vulnerable position (Aanouz

Role of ACE2 receptor and the landscape of treatment options from convalescent plasma therapy to the drug repurposing in COVID-19

Pravindra Kumar¹ · Ashok Kumar Sah² · Greesham Tripathi³ · Anjali Kashyap⁴ · Avantika Tripathi³ · Rashmi Rao¹ · Prabhu C. Mishra³ · Koustav Mallick⁵ · Amjad Husain^{6,7} · Manoj Kumar Kashyap³ 

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Abstract

Since the first case reports in Wuhan, China, the SARS-CoV-2 has caused a pandemic and took lives of > 8,35,000 people globally. This single-stranded RNA virus uses Angiotensin-converting enzyme 2 (ACE2) as a receptor for entry into the host cell. Overexpression of ACE2 is mainly observed in hypertensive, diabetic and heart patients that make them prone to SARS-CoV-2 infection. Mitigations strategies were opted globally by the governments to minimize transmission of SARS-CoV-2 via the implementation of social distancing norms, wearing the facemasks, and spreading awareness using digital platforms. The lack of an approved drug treatment regimen, and non-availability of a vaccine, collectively posed a challenge for mankind to fight against the SARS-CoV-2 pandemic. In this scenario, repurposing of existing drugs and old treatment options like convalescent plasma therapy can be one of the potential alternatives to treat the disease. The drug repurposing provides a selection of drugs based on the scientific rationale and with a shorter cycle of clinical trials, while plasma isolated from COVID-19 recovered patients can be a good source of neutralizing antibody to provide passive immunity. In this review, we provide in-depth analysis on these two approaches currently opted all around the world to treat COVID-19 patients. For this, we used “Boolean Operators” such as AND, OR & NOT to search relevant research articles/reviews from the PUBMED for the repurposed drugs and the convalescent plasma in the COVID-19 treatment. The repurposed drugs like Chloroquine and Hydroxychloroquine, Tenofovir, Remdesivir, Ribavirin, Darunavir, Oseltamivir, Arbidol (Ilfimfenovir), Favi-

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Insights into the biased activity of dextromethorphan and haloperidol towards SARS-CoV-2 NSP6: in silico binding mechanistic analysis. Pandey P, Prasad K, Prakash A*, Kumar V*. *J Mol Med (Berl)*. 2020 Sep 23. doi: 10.1007/s00109-020-01980-1.



Insights into the biased activity of dextromethorphan and haloperidol towards SARS-CoV-2 NSP6: in silico binding mechanistic analysis

Preeti Pandey¹ · Kartikay Prasad² · Amresh Prakash³ · Vijay Kumar²

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Abstract

The outbreak of novel coronavirus disease 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) virus continually led to infect a large population worldwide. SARS-CoV-2 utilizes its NSP6 and Orf9c proteins to interact with sigma receptors that are implicated in lipid remodeling and ER stress response, to infect cells. The drugs targeting the sigma receptors, sigma-1 and sigma-2, have emerged as effective candidates to reduce viral infectivity, and some of them are in clinical trials against COVID-19. The antipsychotic drug, haloperidol, exerts remarkable antiviral activity, but, at the same time, the sigma-1 benzomorphan agonist, dextromethorphan, showed pro-viral activity. To explore the potential mechanisms of biased binding and activity of the two drugs, haloperidol and dextromethorphan towards NSP6, we herein utilized molecular docking-based molecular dynamics simulation studies. Our extensive analysis of the protein-drug interactions, structural and conformational dynamics, residual frustrations, and molecular switches of NSP6-drug complexes indicates that dextromethorphan binding leads to structural destabilization and increase in conformational dynamics and energetic frustrations. On the other hand, the strong binding of haloperidol leads to minimal structural and dynamical perturbations to NSP6. Thus, the structural insights of stronger binding affinity and favorable molecular interactions of haloperidol towards viral NSP6 suggests that haloperidol can be potentially explored as a candidate drug against COVID-19.

Key messages

- Inhibitors of sigma receptors are considered as potent drugs against COVID-19.
- Antipsychotic drug, haloperidol, binds strongly to NSP6 and induces the minimal changes in structure and dynamics of NSP6.
- Dextromethorphan, agonist of sigma receptors, binding leads to overall destabilization of NSP6.
- These two drugs bind with NSP6 differently and also induce differences in the structural and conformational changes that explain their different mechanisms of action.
- Haloperidol can be explored as a candidate drug against COVID-19.

Keywords COVID-19 · NSP6 · Haloperidol · Dextromethorphan · Molecular docking · Molecular dynamics

Electronic supplementary material The online version of this article (<https://doi.org/10.1007/s00109-020-01980-1>) contains supplementary material, which is available to authorized users.

- ✉ Amresh Prakash
aprakash@ggn.amity.edu
- ✉ Vijay Kumar
vkumar33@amity.edu

¹ Department of Chemistry & Biochemistry, University of Oklahoma, 101 Stephenson Parkway, Norman, OK 73019-5251, USA

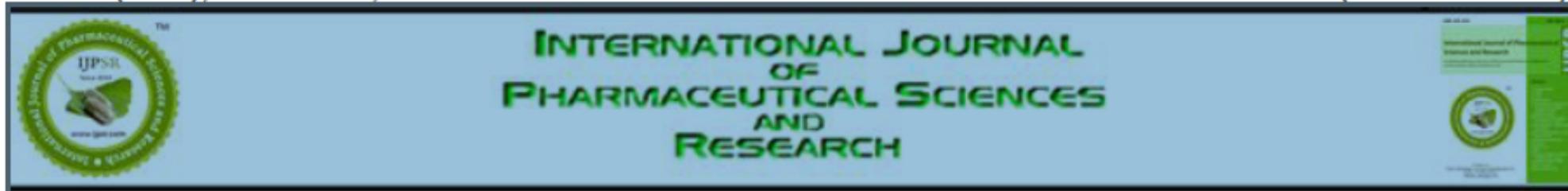
² Amity Institute of Neuropsychology & Neurosciences (AINN), Amity University, Noida, UP 201303, India

³ Amity Institute of Integrative Sciences and Health (AIISH), Amity University Haryana, Gurgaon 122413, India

Introduction

The current outbreak of corona virus disease 2019 (COVID-19) caused by a novel coronavirus SARS-CoV-2 was first reported from Wuhan, China, in late December 2019 [1], which has subsequently affected the entire world, reporting nearly 26 million of confirmed cases of COVID-19 along with ~9.0-lakh deaths as per data recorded in September 1st week, 2020, posing a global threat for human health and economy. With so many novel studies and findings surfaced, since its inception, we are still lagging behind in development of an effective treatment strategy to control the virus spread and prevent the disease [2–7].

ABSTRACT: The outbreak of novel coronavirus disease 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus-2 (SARSCoV-2) virus continually led to infect a large population worldwide. SARS-CoV-2 utilizes its NSP6 and Orf9c proteins to interact with sigma receptors that are implicated in lipid remodeling and ER stress response, to infect cells. The drugs targeting the sigma receptors, sigma-1 and sigma-2, have emerged as effective candidates to reduce viral infectivity, and some of them are in clinical trials against COVID-19. The antipsychotic drug, haloperidol, exerts remarkable antiviral activity, but, at the same time, the sigma-1 benzomorphan agonist, dextromethorphan, showed pro-viral activity. To explore the potential mechanisms of biased binding and activity of the two drugs, haloperidol and dextromethorphan towards NSP6, we herein utilized molecular docking-based molecular dynamics simulation studies. Our extensive analysis of the protein-drug interactions, structural and conformational dynamics, residual frustrations, and molecular switches of NSP6-drug complexes indicates that dextromethorphan binding leads to structural destabilization and increase in conformational dynamics and energetic frustrations. On the other hand, the strong binding of haloperidol leads to minimal structural and dynamical perturbations to NSP6. Thus, the structural insights of stronger binding affinity and favorable molecular interactions of haloperidol towards viral NSP6 suggests that haloperidol can be potentially explored as a candidate drug against COVID-19.



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MANAGEMENT AGAINST COVID-19 THROUGH NUTRITIONAL SUPPLEMENTATION TO BUILD ADAPTIVE IMMUNITY - A SYSTEMATIC REVIEW

Luxita Sharma

Dietetics and Applied Nutrition, Gurugram - 122002, Haryana, India.

Keywords:

COVID-19, Adaptive Immunity,
Nutrition, Vitamins, Minerals,
Immune system

Correspondence to Author:

Luxita Sharma

Associate Professor,
Dietetics and Applied Nutrition,
Gurugram - 122002, Haryana, India.

E-mail: lakshita1982@gmail.com

ABSTRACT: As humanity is progressing, many new borne infections are borne, and the stability and efficiency of the human body are being tested. Today the World is fighting with a deadly Novel infection named Corona Virus Disease. The aim of this systematic review is to find out the efficacy of Nutritional Interventions against the infections caused in the body due to pathogens. Further, the recommendations can be made for further researches based on the evidence collected. To collect the data, electronic databases such as Scopus, Pub Med, NCBI, and web of science have been used. The peer-reviewed journals and newspaper reports are being cited with the English language. The papers were published from 1989 to 2020. Finally, a total of twelve studies were identified, and the pathways of all nutrient metabolisms are included in the study. The studies were mostly carried out in Asian and European countries on human as well as animals. All the studies except one supported the role of Nutrients in preventing and curing the infection caused by pathogens such as





Identification of potential inhibitors against SARS-CoV-2 by targeting proteins responsible for envelope formation and virion assembly using docking based virtual screening, and pharmacokinetics approaches. Bhowmik D, Nandi R, Jagadeesan R, Kumar N, **Prakash A**, Kumar D. *Infect Genet Evol.* 2020 Jul 5; 84:104451. doi: 10.1016/j.meegid.2020.104451.

ABSTRACT: WHO has declared the outbreak of COVID-19 as a public health emergency of international concern. The evergrowing new cases have called for an urgent emergency for specific anti-COVID-19 drugs. Three structural proteins (Membrane, Envelope and Nucleocapsid protein) play an essential role in the assembly and formation of the infectious virion particles. Thus, the present study was designed to identify potential drug candidates from the unique collection of 548 anti-viral compounds (natural and synthetic anti-viral), which target SARS-CoV-2 structural proteins. High-end molecular docking analysis was performed to characterize the binding affinity of the selected drugs-the ligand, with the SARS-CoV-2 structural proteins, while high-level Simulation studies analyzed the stability of drug-protein interactions. The present study identified rutin, a bioflavonoid and the antibiotic, doxycycline, as the most potent inhibitor of SARS-CoV-2 envelope protein. Caffeic acid and ferulic acid were found to inhibit SARS-CoV-2 membrane protein while the anti-viral agent's simeprevir and grazoprevir showed a high binding affinity for nucleocapsid protein. All these compounds not only showed excellent pharmacokinetic properties, absorption, metabolism, minimal toxicity and bioavailability but were also remain stabilized at the active site of proteins during the MD simulation. Thus, the identified lead compounds may act as potential molecules for the development of effective drugs against SARS-CoV-2 by inhibiting the envelope formation, virion assembly and viral pathogenesis.



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Research Paper

Identification of potential inhibitors against SARS-CoV-2 by targeting proteins responsible for envelope formation and virion assembly using docking based virtual screening, and pharmacokinetics approaches

Deep Bhowmik^a, Rajat Nandi^a, Rahul Jagadeesan^b, Niranjan Kumar^c, Amresh Prakash^d, Diwakar Kumar^{a,*}

^a Department of Microbiology, Assam University, Silchar 788011, Assam, India

^b CAS in Crystallography and Biophysics, Guindy Campus, University of Madras, Chennai 600025, India

^c School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi 110067, India

^d Amity Institute of Integrative Sciences and Health, Amity University Haryana, Gurgaon 122413, India



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ABSTRACT

WHO has declared the outbreak of COVID-19 as a public health emergency of international concern. The evergrowing new cases have called for an urgent emergency for specific anti-COVID-19 drugs. Three structural proteins (Membrane, Envelope and Nucleocapsid protein) play an essential role in the assembly and formation of the infectious virion particles. Thus, the present study was designed to identify potential drug candidates from the unique collection of 548 anti-viral compounds (natural and synthetic anti-viral), which target SARS-CoV-2 structural proteins. High-end molecular docking analysis was performed to characterize the binding affinity of the selected drugs-the ligand, with the SARS-CoV-2 structural proteins, while high-level Simulation studies analyzed the stability of drug-protein interactions. The present study identified rutin, a bioflavonoid and the antibiotic, doxycycline, as the most potent inhibitor of SARS-CoV-2 envelope protein. Caffeic acid and ferulic acid were found to inhibit SARS-CoV-2 membrane protein while the anti-viral agent's simeprevir and grazoprevir showed a high binding affinity for nucleocapsid protein. All these compounds not only showed excellent pharmacokinetic properties, absorption, metabolism, minimal toxicity and bioavailability but were also remain stabilized at the active site of proteins during the MD simulation. Thus, the identified lead compounds may act as potential molecules for the development of effective drugs against SARS-CoV-2 by inhibiting the envelope formation, virion assembly and viral pathogenesis.

1. Introduction

On 31st December 2019, China revealed to the world health organization (WHO) and the rest of the world, the occurrence of symptoms of unexplained pneumonia in a cluster of cases from Wuhan city (Rodríguez-Morales et al., 2020; Zhou et al., 2020a). The causative agent was later identified as a novel strain of coronavirus, named as 2019-nCoV and the disease as COVID-19 (Zhou et al., 2020a). On 30th January 2020, WHO declared the outbreak of COVID-19 as a public health emergency of international concern and also called a pandemic. The 2019-nCoV shared a 79.5% sequence identity to SARS-CoV. Recently, the Coronaviridae Study Group (CSG) of the International Committee on Taxonomy of Viruses (ICTV) renamed it SARS-CoV-2 (Coronaviridae Study Group of the International Committee on

Taxonomy of Viruses, 2020). The ever-growing infections and the mortality rate across the globe have called an urgent emergency for specific anti-COVID-19 therapeutics and extensive screening of presently available drugs for the treatment and prevention of SARS-CoV-2. Coronaviruses (CoVs) are enveloped positive-stranded RNA viruses and Coronaviridae can be subdivided into four groups- *alpha*-, *beta*-, *gamma*- and *delta*- CoV (Perlman and Netland, 2009; Fehr and Perlman, 2015). Members of this virus family infect the mammalian respiratory organ from the upper respiratory tract (URTIs) to the lower respiratory tract (LRTIs) and gastrointestinal tract by incompletely understood mechanisms (Fehr and Perlman, 2015; Cong and Ren, 2014). SARS-CoV-2 is the seventh-known SARS virus that will infect people after 229E, NL63, OC43, HKU1, MERS-CoV and the original SARS-CoV (Zhu et al., 2020). SARS-CoV-2 is a member of the subgenus Sarbecovirus (beta-

A low cost portable microfluidics embedded on chip rRT-PCR and microelectrode array coupled point-of care optoelectronic device for large scale screening of emerging viral disease like SARS COV2

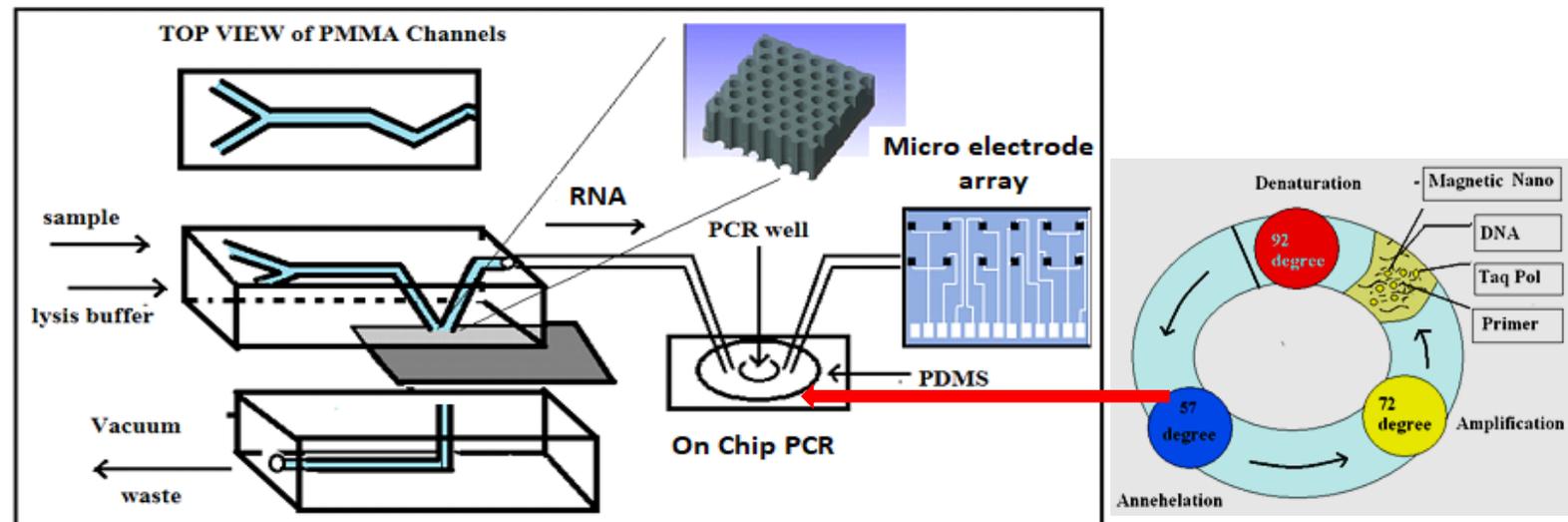
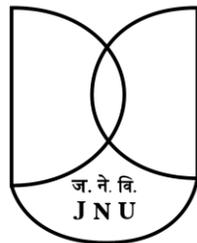


Recent outbreak of Coronavirus disease (Covid-19) has contributed to a significant public health concern and made a huge impact in our lives. An RT PCR based detection system is the key for the detection of disease. But it requires high end laboratory equipment, trained personnel, analysis of data and thus becomes time consuming.

To deal with this emergency, a portable, low cost, low voltage operated, printed heater based *on-chip* spatial PCR, integrated with the *in-built* optoelectronic detection system had been designed for large scale screening of COVID 19.



Dr. Ranjita Ghosh
Moulick (PI)



Dietary management to build adaptive immunity against COVID-19

Luxita Sharma*

Department of Dietetics and Applied Nutrition, Amity University, Gurgaon – 122413, India.

Abstract: Today's technology laced world progression has given a setback to human health. The world has faced the adversity of many new borne deadly pathogens such as Ebola, SARS, MERS and COVID-19. The human body has inherent and adaptive immunity which fights back with pathogens. Mostly the adaptive immunity is built by vaccinations or certain medications. But many research outcomes have shown that a diet filled with nutrients and right choices of food can help to build adaptive immunity. Micronutrients such as vitamins A, C, D, E, B2, B6, and B12, folic acid, iron, selenium, and zinc are important for avoiding pathogens attacks on human body. The deficiencies prevailing in body could be improved by supplementation of nutrients in accordance to recommended dietary allowances will help strengthen the immune system in return. We presently know only diet is not sufficient in fighting against pathogen attacks but the role of diet cannot be ignored in controlling infections. In this scenario, this review aims at summarizing those studies which demonstrated that supplementation of above micronutrients can help fight COVID-19 in specific.

Keywords: COVID 19, Adaptive Immunity, Nutrition, Vitamins, Minerals.

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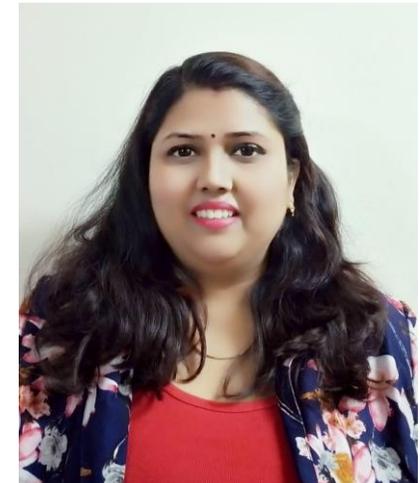
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Immunomodulatory effect and supportive role of traditional herbs, spices and nutrients in management of COVID-19

Luxita Sharma*

Department of Dietetics and Applied Nutrition, Amity University, Gurgaon – 122413, India.

Abstract: Coronavirus disease 2019 (COVID-19) caused by SARS-CoV-2 is a new strain of coronavirus that causes respiratory illnesses with a start of flu like symptoms. This disease can be fatal and is already spread all over the world, making World Health Organization to declare it as a pandemic. Researchers from across globe are working tirelessly around the clock to find vaccine or a cure. In the view of the pandemic many treatments are being tried on the patients and various treatment modalities are being followed including traditional medicine which has shown promising results in managing this disease. The traditional medicines include the use of herbs, nutrition and spices that are widely available and used in day to day life by majority of Asian population. In this paper the role of various herbs and spices such as Oregano, Ashwagandha, Ginseng, Basil, Sage, Curcumin, Fenugreek, Ginger and Garlic in building immunity against pathogenic invasions based on researches based evidence has been compiled and reviewed. Since there is no cure available for COVID-19 till now, supportive therapy is playing a major role in managing this pandemic. The AYUSH ministry has also promoted the use of above herbs for a patient suffering from COVID-19. The corona virus is present in respiratory system as shown by different studies and it has different strains. The guidelines laid by the ICMR and WHO shows that use of herbs, spices and nutrients can be helpful to manage this virus by increasing the immunity in patients. Note that we are not claiming any cures but the herbs and spices used in day to day life are very much effective in management of COVID-19. World Health Organization (WHO) has recognized the use of alternative and traditional medicine in the management of COVID-19 but the herbs should be used in prescribed amounts and overdose of them can be harmful for health. Therefore the present article will enlighten the readers about the role of herbs, spices and nutrients in managing COVID-19.





Clinical Linkage of COVID-19 with Hypertension, Diabetes and Cardiovascular Disease

Bimal Chhajer¹, Vikram Singh^{*2}, Girija Kumari³

¹Department of Preventive Cardiology, SAAOL Heart Center, Farm No. 5, DLF Westend, Mandi Road, Chhattarpur, New Delhi-110030, Delhi, India

²Department of Medical Laboratory Technology, Amity Medical School, Amity University Haryana, Amity Education Valley Gurugram, Panchgaon, Manesar-122412, Haryana, India

³Department of Clinical Research, Amity Medical School, Amity University Haryana, Amity Education Valley Gurugram, Panchgaon, Manesar-122412, Haryana, India

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Treatment

ABSTRACT

The coronavirus outbreak caused by the pandemic Coronavirus Disease (COVID-19) is heart-rending millions live around the globe, and it is the foremost major human tragedy in history. World Health Organization (WHO) declared the coronavirus disease (COVID-19) a pandemic and global outbreak with a severe public health concern. This outbreak caused by a novel infectious coronavirus of Severe Acute Respiratory Syndrome Coronavirus- 2 (SARS-CoV-2) sequences leading to an emergent crisis with significant loss of health and global economy. COVID-19 is more prone to exacerbate health concerns in hypertensive, diabetes, and cardiovascular disease patients, however, COVID-19 incidence outcomes are inconsistent. Prevention and control of the outbreak are very challenging due to the complex nature of the virus and its pathogenesis. WHO, CDC, and every national health authority are taking necessary actions to combat the contagious novel infection. The purpose of the review is to discuss potential mechanisms and clinical linkages between high blood pressure, diabetes, cardiovascular diseases, and SARS-CoV-2. We hope that we can identify information deficiencies that need more review and clinical evidence of the COVID-19 for hypertension and cardiovascular problems in patients with diabetes. This article will provide a comprehensive integrative strategy to control and manage of current outbreak and related mortality around the world.





Development of on-spot diagnostic kit for COVID-19 based on RT-LAMP integrated CRISPR-Cas technique



PI: Dr. Saif Hameed, Amity University Haryana, Gurugram



Co-Investigators (CI):

Dr. Zeeshan Fatima, Amity University Haryana, Gurugram

Dr. Munindra Ruwali, Amity University Haryana, Gurugram

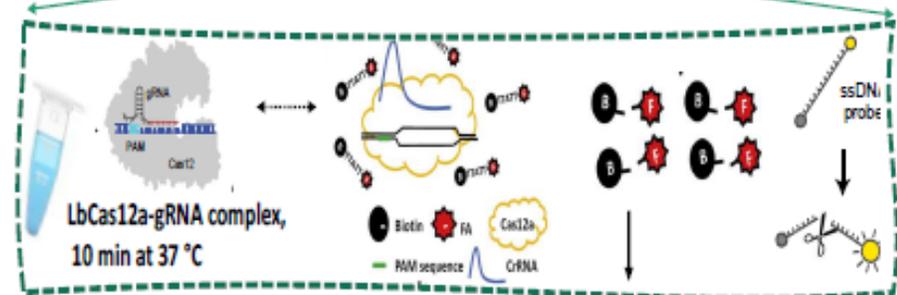
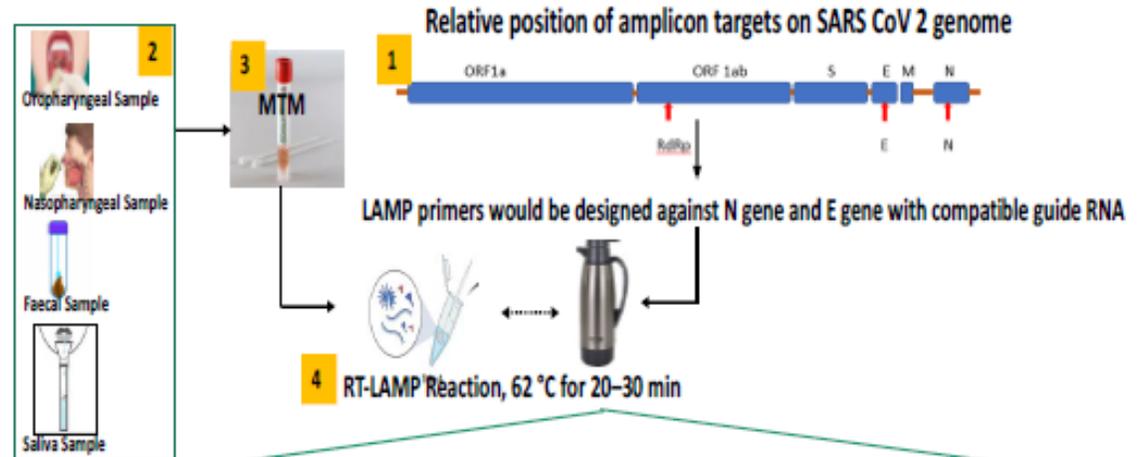
Dr. Ashok Rattan, PathKind Labs, Gurugram

Principal collaborator (PC):

Dr. Devashish Rath, BRNS-BARC, Mumbai

Duration: 12 months

Total Budget: 16,56,550 INR



- **Rapid:** The RT-LAMP and CRISPR-Cas12 reaction takes less than 1 hour.
- **Specific:** Because detection depends on the identification and subsequent cleavage of SARS-CoV-2 genomic sequences by the Cas12 enzyme.
- **Sensitive:** Because of the integration of two techniques.
- **Field-deployable:** No sophisticated equipment is required.
- **Easy to use:** The colorimetric reaction coupled to lateral flow read out facilitate easy visual inspection of the results.
- **Adaptability:** The developed method can be easily adjusted for detection of other emerging pathogens.

Identifying the natural polyphenol catechin as a multi-targeted agent against SARS-CoV-2 for the plausible therapy of COVID-19: an integrated computational approach

Chandra Bhushan Mishra[†], Preeti Pandey[†], Ravi Datta Sharma[†],
Md. Zubair Malik, Raj Kumar Mongre, Andrew M. Lynn, Rajendra Prasad,
Raok Jeon and Amresh Prakash 

Corresponding authors: Amresh Prakash, Amity Institute of Integrative Sciences and Health (AIISH), Amity University Haryana, Gurgaon 122413, India. E-mail: amreshprakash@jnu.ac.in, aprakash@ggn.amity.edu; Raok Jeon, College of Pharmacy, Sookmyung Women's University, Cheongpa-ro 47-gil 100, Yongsan-gu, Seoul, 04310, Republic of Korea. E-mail: rjeon@sookmyung.ac.kr

[†]These authors contributed equally to this work.

Abstract

The global pandemic crisis, coronavirus disease 2019 (COVID-19), caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has claimed the lives of millions of people across the world. Development and testing of anti-SARS-CoV-2 drugs or vaccines have not turned to be realistic within the timeframe needed to combat this pandemic. Here, we report a comprehensive computational approach to identify the multi-targeted drug molecules against the

Invention : **An Antimicrobial Face Mask Using Nanoparticle Coating**

Patent Application No. 202011017740 filed in India on 25/04/2020



INVENTORS

Arvind Chhabra, AUH

Monika Vats, AUH

Neha Kuhar, AUH

Shatendra K. Sharma, AUH

ABSTRACT OF INVENTION

We have developed a three-layered reusable, biodegradable, anti-microbial face mask. The middle layer is coated with nanoparticles exhibiting anti-microbial properties. The two layered scaffolds will house the middle layer, which could be used with washing or replaced with new filtration assembly. The face-masks that are in use today are either surgical masks that do not protect against infectious agents or are not reusable, and leave carbon foot print on the environment. Further, the masks thrown in trash by asymptomatic patients could further contribute in spread of the virus. The face mask we have developed is reusable, biodegradable, and has anti-microbial properties. It could also be upgraded to N95 grade and can be used to filter out particulate materials to protect against air pollutants.



Targeting virus-host interaction by novel pyrimidine derivative: an in-silico approach towards discovery of potential drug against COVID-19.

Rane JS, Pandey P, Chatterjee A, Khan R, Kumar A, Prakash A*, Ray S*. *J Biomol Struct Dyn.* 2020 Jul 20:1-11. doi: 10.1080/07391102.2020.1794969.

ABSTRACT: The entire human population over the globe is currently facing appalling conditions due to the spread of infection from coronavirus disease-2019 (COVID-19). The spike glycoprotein of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) present on the surface of the virion mediates the virus entry into the host cells and therefore is targeted by several scientific groups as a novel drug target site. The spike glycoprotein binds to the human angiotensin-converting enzyme-2 (hACE2) cell surface receptor abundantly expressed in lung tissues, and this binding phenomenon is a primary determinant of cell tropism and pathogenesis. The binding and internalization of the virus is the primary and most crucial step in the process of infection, and therefore the molecules targeting the inhibition of this process certainly hold a significant therapeutic value. Thus, we systematically applied the computational techniques to identify the plausible inhibitor from a chosen set of well characterized diaryl pyrimidine analogues which may disrupt interfacial interaction of spike glycoprotein (S) at the surface of hACE2. Using molecular docking, molecular dynamics (MD) simulation and binding free energy calculation, we have identified AP-NP (2-(2-amino-5-(naphthalen-2-yl)pyrimidin-4-yl)phenol), AP-3-OMe-Ph (2-(2-amino-5-(3-methoxyphenyl)pyrimidin-4-yl)phenol) and AP-4-Me-Ph (2-(2-amino-5-(p-tolyl) pyrimidin-4-yl)phenol) from a group of diaryl pyrimidine derivatives which appears to bind at the interface of the hACE2-S complex with low binding free energy. Thus, pyrimidine derivative AP-NP may be explored as an effective inhibitor for hACE2-S complex. Furthermore, *in vitro* and *in vivo* studies will strengthen the use of these inhibitors as suitable drug candidates against SARS-COV-2.

Targeting virus–host interaction by novel pyrimidine derivative: an *in silico* approach towards discovery of potential drug against COVID-19

Jitendra Subhash Rane^{a#}, Preeti Pandey^{b#}, Aroni Chatterjee^c, Rajni Khan^d, Abhijeet Kumar^e , Amresh Prakash^f  and Shashikant Ray^g 

^aDepartment of Biosciences & Bioengineering, Indian Institute of Technology Bombay, Mumbai, India; ^bDepartment of Chemistry & Biochemistry, University of Oklahoma, Norman, OK, USA; ^cIndian Council of Medical Research (ICMR)—Virus Research Laboratory, NICED, Kolkata, India; ^dMotihari College of Engineering, Motihari, India; ^eDepartment of Chemistry, Mahatma Gandhi Central University, Motihari, India; ^fAmity Institute of Integrative Sciences and Health, Amity University Haryana, Gurgaon, India; ^gDepartment of Biotechnology, Mahatma Gandhi Central University, Motihari, India

Communicated by Ramaswamy H. Sarma

ABSTRACT

The entire human population over the globe is currently facing appalling conditions due to the spread of infection from coronavirus disease-2019 (COVID-19). The spike glycoprotein of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) present on the surface of the virion mediates the virus entry into the host cells and therefore is targeted by several scientific groups as a novel drug target site. The spike glycoprotein binds to the human angiotensin-converting enzyme-2 (hACE2) cell surface receptor abundantly expressed in lung tissues, and this binding phenomenon is a primary determinant of cell tropism and pathogenesis. The binding and internalization of the virus is the primary and most crucial step in the process of infection, and therefore the molecules targeting the inhibition of this process certainly hold a significant therapeutic value. Thus, we systematically applied the computational techniques to identify the plausible inhibitor from a chosen set of well characterized diaryl pyrimidine analogues which may disrupt interfacial interaction of spike glycoprotein (S) at the surface of hACE2. Using molecular docking, molecular dynamics (MD) simulation and binding free energy calculation, we have identified AP-NP (2-(2-amino-5-(naphthalen-2-yl)pyrimidin-4-yl)phenol), AP-3-OMe-Ph (2-(2-amino-5-(3-methoxyphenyl)pyrimidin-4-yl)phenol) and AP-4-Me-Ph (2-(2-amino-5-(p-tolyl) pyrimidin-4-yl)phenol) from a group of diaryl pyrimidine derivatives which appears to bind at the interface of the hACE2-S complex with low binding free energy. Thus, pyrimidine derivative AP-NP may be explored as an effective inhibitor for hACE2-S complex. Furthermore, *in vitro* and *in vivo* studies will strengthen the use of these inhibitors as suitable drug candidates against SARS-COV-2.

Abbreviations: 6-HB: six-helix bundle; ADME: absorption, distribution, metabolism and excretion; AP-NP: 2-(2-amino-5-(naphthalen-2-yl)pyrimidin-4-yl) phenol; AP-4-Me-Ph: 2-(2-amino-5-(p-tolyl)pyrimidin-4-yl) phenol; AP-3-OMe-Ph: 2-(2-amino-5-(3-methoxyphenyl)pyrimidin-4-yl) phenol; COVID-19: coronavirus disease 2019; CQ: chloroquine; hACE2: human angiotensin converting enzyme-2; hACE2-S protein complex: human angiotensin converting enzyme-2 receptor and severe acute respiratory syndrome coronavirus 2 spike protein complex; HR1: heptad repeat 1; HR2: heptad repeat 2; PDB: protein data bank; RBD: receptor-binding domain; SARS-CoV-2S: severe acute respiratory syndrome coronavirus 2 spike protein; TMPRSS-2: transmembrane protease serine 2

ARTICLE HISTORY

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KEYWORDS

hACE2; receptor;
coronavirus; pyrimidine
derivatives; binding site

1. Introduction

The world is currently going through a debilitating phase of acute health disaster attributed to the global pandemic brought about by the novel coronavirus disease-2019 (COVID-19) (Enayatkhani et al., 2020; Joshi et al., 2020; Kirchdoerfer et al., 2016; Muralidharan et al., 2020). Sequencing and simultaneous phylogenetic identification of the virus responsible for COVID-19 confirmed that it as a

novel β -coronavirus that shared 88% sequence identity with two bat-derived SARS-like coronaviruses (Lu et al., 2020; Pant et al., 2020; Wang et al., 2020). Additionally, it was shown that this coronavirus (CoV), termed as 2019-nCoV (Elfiky, 2020; Gorbalenya et al., 2020), shared 79.5% sequence identity with SARS-CoV (Elfiky & Zazzam, 2020; Lu et al., 2020; Wang et al., 2020; Xia et al., 2020) which caused the severe acute respiratory syndrome pandemic in 2012. Therefore, this newly identified virus was called as SARS-CoV-2 (Aanouz

E- BANKING SERVICES AND CUSTOMER SATISFACTION IN COVID-19- A CASE STUDY OF MANESAR CITY BANKS

Dr. Nilmani Tripathi¹, Nidhi Ahuja², Varsha Yadav³, Vishala Raghav⁴

The Declaration of the authors for publication of Research Paper in Anvishiki: International Journal of Research ISSN 0973-9777 Six monthly Journal of all Research: We, Dr. Nilmani Tripathi¹, Nidhi Ahuja, Varsha Yadav, Vishala Rag the authors of the research paper entitled E- BANKING SERVICES AND CUSTOMER SATISFACTION IN COVID-19- A CASE STUDY OF MANESAR CITY BANKS declare that, We take the responsibility of the content and material of our paper as We ourself have written it and also have read the manuscript of our paper carefully. Also, We hereby give our consent to publish our paper in Anvishiki Journal . This research paper is our original work and no part of it or it's similar version is published or has been sent for publication anywhere else. We authorise the Editorial Board of the Journal to modify and edit the manuscript. We also give our consent to the Editor of Anvishiki Journal to own the copyright of our research paper.

Abstract: - *Global pandemic due to COVID - 19 has changed the way of business now a days. Every business now a days has almost adopted online mode of business. This had provided a lot of opportunities together with threats to the organization. The banking sector in the Indian economy, which had adopted the online mode of providing services in late 80s with a view of providing more satisfaction to the customers, is in a win-win situation during this pandemic as most of the services are online. The present paper tries to examine the satisfaction level among the selected banks. The study shows there is a significant relationship between the variables taken in the study as well as there is difference in satisfaction of customers in selected banks.*

Impact of Covid 19 - A Study of the Major Stressors and Coping Strategies.

CA. Kamakshi Mehta,

Assistant Professor at Amity University, Haryana, India

Dr. Shikha Sharma,

Assistant Professor at Amity University, Haryana, India

Abstract

The current outbreak of COVID – 19, corona virus from the SARS family, is a respiratory disease highly infectious in nature. With its epic centre at Wuhan a province in China. The virus has spread its wings all around the globe with major deadly impact on the developed countries where the death toll has been the maximum. The deadly virus has not only taken up the lives of the humans but also has put stigma on the lives of living people as well. It has resulted to a steep rise in the level of stress which is playing a toll on the mental health of the humans of all age groups in all the impacted countries. The present study also puts forth the major coping strategies like meditation, financial assistance from the government etc. which can be used to combat these stressors which are an outcome of the terrorizing COVID – 19 infection.

COVID-19 : A nightmare for the Indian Economy

1. **CA .Kamakshi Mehta** is an Assistant Professor at Amity University , Haryana, India
2. **Mr Shiv Swaroop Jha** is an Assistant Professor at Amity University, Haryana , India

Abstract

The objective of our study is to conduct and accomplish a retrospective analysis of the macro-economic repercussions of the various Pandemics which have emerged till date and also to forecast the impact of Covid -19 on the Indian Economy. Covid -19 is a contagious disease belonging to the SARS COV-2 family . The best method recommended to restrain the virus is by social distancing and self-isolation . The major method being used by infected countries is complete lock down . This method may help in containing the virus spread but it is paving the way to the Global recession which will have a severe consequence on all sectors of the economy and all the countries-be it developed or developing . We also suggest that additional work is

A STUDY OF THE IMPACT OF COVID-19 ON BUYING BEHAVIOUR OF CONSUMERS .

Dr. Shikha Sharma*
CA. Kamakshi Mehta**

ABSTRACT

December 2019, "The Black date" written boldly in the global history, a month which shall be remembered for many generations to come. The year 2019 has seen a death count which has outnumbered even the death count of World WarII. In the early part of December 2019, the city of Wuhan, China witnessed an outbreak of a deadly disease Corona virus 2 (SARS- COV-2). The virus has spread its wings all around the globe with major deadly impact on the developed countries where the death toll has been the maximum. The perceived risk of contracting the disease has led to a massive scare in the human mind leading to various control and preventive measures being taken up. The pandemic has made a significant psychosocial impact on the behaviour of the people towards their buying needs. The changes in the priorities have been noticed in the people's buying choices due to the fear of the uncertainties caused by the disease. The present research studies, the degree of impact of various independent variables such as Change in Shopping habits, Increase in Online Shopping, Reduction in purchasing capacity as independent variable on buying behaviour as dependent variable. i.e. buying behaviour of the respondents. The study, using primary data sources of 250 respondents which were collected by questionnaire using google forms. The non parametric statistical tool i.e. multiple regression has been used to analyse the relationship between dependent variable and independent variables. The results of the research clearly indicate that there is significant impact of fear of disease, job insecurity, and medical expenditure on the buying behaviour of the respondents.

Keywords : Covid-19, Buying Behaviour, Outbreak, Consumers.