







15-16 May 2021

16:00 PM to 19:30 PM (IST) UTC/GMT

RECENT PROGRESS IN BIOACTIVE COMPOUNDS & MOLECULES AGAINST RESPIRATORY DISEASES AND COMORBIDITIES: THERANOSTICS AND FUTURE CHALLENGES

The 2nd HeriCure-Ukzn: AHybrid International Conference and Webinar

Recent Progress in Bioactive Compounds & Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges

15-16 May, 2021

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Message from Organizing Secretary



Dr. Dileep Tiwari

Chairman & Chief Organizer

Founder & C.E.O.,

Hericure Healthcare Ltd, 306-B, Zen Business Center, NR Bhumkar Chowk, (Hinjewadi)-Wakad, Pune, (India). Hon. Scientist, Catalysis Peptide & Research Unit, School of Health Science, University of KwaZulu-Natal, Durban (South Africa).

Today, we all are here by the grace of God, we all are gathered here to inspire, innovate and engage with scientific platforms in which various researchers, scientists,

academicians, and industrialists earning their valuable time to provide a unique shape and infrastructure to the society. Today, we all have a common objective, which is to find out solutions for global threatening issues. Our serene environment in this era had affected all the cores and the entire biosphere is paying a huge cost for that. God's biggest discovery, humans, who are severely affected and losing their lives through natural or materialistic calamities. We as a human-beings know that various phenomena occurring on earth right now are not in our hands, but we have something, that can prevent the rising of various disasters. And with respect to this today we came together to present our self on a common platform where we discuss and rediscover research on "Recent Progress in Bioactive Compounds & Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges". When we say, diseases then the first thing that should come to our mind that is prevention, and for that whatever research, protocols, and strategies were defined or going to be formed becomes the part of phenomenal existence. The topic, on which the entire conference will be surrounded is known to be novel drug/bioactive compounds. Therefore, the discovery and applications of novel natural bioactive compounds can be exploited as new opportunities to control these diseases in the modern era of antibiotic resistance and the emergence of new strains of pathogens. I, believe that these 2 days of the international conference i.e., 15 and 16 May becomes remarkable and can be helpful in rebuilding our beautiful society by choosing natural pathways of living a life. Once again, I would like to thank all eminent personalities for making this conference a successful one.

Message from President of Conference



Prof. Anil A Chuturgoon

Dean of Research (Acting), College of Health Sciences, University of KwaZulu-Natal, Durban (South Africa)

I am sure that the international conference, which will be held on May 15th and 16th, will be memorable and will contribute to the restoration of our beautiful society through the adoption of natural living practices. I'd want to thank everyone who helped

make this conference a success once more. I congratulate you and send my best wishes for the conference's success. The mission of this global conference is to inspire, build, and connect with intellectual platforms in which a varied group of researchers, scientists, academics, and business leaders are investing substantial time and effort to give society a particular shape and infrastructure. Today, we are all working towards the same goal: finding solutions to the world's most serious issues. The goal of this worldwide conference is to inspire, build, and connect with scientific platforms where a diverse group of researchers, scientists, academics, and industry leaders are putting in major effort to give society a particular shape and infrastructure. Such conferences play a significant role for reenergizing scientific communities the scientific community is made up of many different types of scientists who engage with one another. There are several "sub-communities" focusing on specific scientific subjects and within certain institutions, as well as multidisciplinary and cross-institutional activity. The theme focusing biomolecules, either natural-derived/-based biomolecules have played an increasingly essential role in innovative drug discovery (as a prototype drug template) for prospective chronic illness treatment throughout the last decade. Many recent studies have shown that developing natural peptide/protein-based, toxin-based, and antibodybased medications can increase the biomedical efficiency of disease-specific therapy greatly. I believe that this conference is going to help in exploration, expansion and endeavour new researchers so that their innovative ideas can help in creating a scientific platform.

Message from Organizing Secretary



Dr. Divakar Sharma, Hericure HealthCare Ltd, Pune (India)

The objective of this international conference is to inspire, create, and engage with scientific platforms in which diverse researchers, scientists, academics, and industrialists are investing their significant time to bring a distinctive shape and infrastructure to society. Today,

we all have a same goal: to find solutions to the world's most pressing problems. Our peaceful atmosphere in this era has had an impact on all cores, and the entire biosphere is paying a high price as a result. God's greatest discovery: "people" who are adversely impacted and die as a result of natural or materialistic disasters. We, as humans, recognize that we have no control over the current events on the planet, but we do have control over something that can prevent tragedies from occurring. In light of this, we have gathered today to offer ourselves on a shared platform where we can talk and rediscover research on "Recent Progress in Bioactive Compounds and Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges" When we think of diseases, the first thing that comes to mind is prevention, and whatever studies, protocols, and methods have been specified or are being developed for that purpose have become part of our existence. I trust that these two days of the international conference, on the 15th and 16th of May, will be memorable and will contribute to the reconstruction of our beautiful society by adopting natural methods of life. I'd want to thank all of the distinguished individuals who contributed to the success of this conference once again.

Message from Convener Scientific and Secretarial Committee



Dr. D R Bharadwaj

Head, Dept. of Life Sciences RPS Degree College, Mahendergarh, Haryana (India)

The goal of this worldwide conference is to inspire, build, and connect with scientific platforms where a diverse group of

researchers, scientists, academics, and business leaders are putting in major effort to give society a particular shape and infrastructure. Today, we are all working toward the same goal: finding solutions to the world's most serious issues. Our peaceful period has had an impact on all cores, and the biosphere as a whole is paying a heavy price as a result. God's greatest discovery: "humans" who are negatively influenced by natural or materialistic tragedies and perish as a result. We acknowledge that we have no power over current happenings on the earth, but we do have power over something that can avoid disasters. As a result, we've come today to share a common platform where we can discuss and rediscover research on "Recent Progress in Bioactive Compounds and Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges." When we think about diseases, the first thing that comes to mind is prevention, and any research, protocols, or procedures which have been specified or are being developed for that reason have become a part of our everyday lives. I am confident that the international conference, which will take place on the 15th and 16th of May, will be unforgettable and will contribute to the restoration of our beautiful society through the adoption of natural living practices. Once again, I'd want to express my gratitude to all of the remarkable persons who contributed to the success of this conference.



Prof. Gert H Kruger

Professor, CPRU School of Health Sciences, University of KwaZulu-Natal, Durban (South Africa)

I am convinced that the international conference, which will be held on the 15th and 16th of May, will be memorable and will contribute

to the restoration of our beautiful society by promoting natural living habits. Once again, I'd like to convey my gratitude to all of the extraordinary people who helped make this conference a success. The purpose of this global conference is to inspire, establish, and connect with scientific platforms where a varied set of researchers, scientists, academics, and business leaders are working hard to shape and infrastructure society. We've gathered today to discuss and rediscover research on "Recent Progress in Bioactive Compounds and Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges," where technical people can debate subjects like the significance of biomolecules in infectious illness treatment. I congratulate and give my best wishes for the success of this conference.

Message from Convener Scientific and Secretarial Committee



Prof. Tricia Naicker

CPRU, Discipline of Pharmaceutical Sciences, University of KwaZulu-Natal, Durban (South Africa)

I am confident that the worldwide conference, which will take place on the 15th and 16th of May, will be unforgettable and will help to restore our beautiful society by encouraging natural living habits. Once again, I'd like to express my gratitude to all of the outstanding people who contributed to the success of this conference. The goal of

this international conference is to inspire, build, and connect with scientific platforms where a diverse group of researchers, scientists, academics, and business executives are hard at work shaping and constructing society. I extend my congratulations and best wishes for the conference's success.

Message from Distinguished Guests and Speakers



Prof. B. NCAMA

Deputy Vice Chancellor

UKZN, Durban, (SA)

I'm sure that the overall gathering, which will happen on the fifteenth and sixteenth of May, will be remarkable and will assist with re-establishing our delightful society by empowering common living propensities. By and by, I'd prefer to offer my thanks to the

entirety of the remarkable individuals who added to the accomplishment of this meeting. The objective of this worldwide conference is to move, fabricate, and interface with logical stages where an assorted gathering of analysts, researchers, scholastics, and business chiefs are working diligently forming and developing society. I broaden my congrats and all the best for the conference's prosperity.

Message from Distinguished Guests and Speakers



Professor Fernando Albericio

Professor, Department of Chemistry, College of Agriculture, Engineering and Science, UKZN, Durban (South Africa) & University of Barcelona (Spain)

I express my gratitude and warm regards to all elite members of conference who had created a dynamic, flexible, innovative and technical platform for all of us. I am happy to serve this international

conference. I'm confident that the overall gathering, which will take place on May 15th and 16th, will be amazing and will aid in the re-establishment of our pleasant society by supporting common living proclivities. The goal of this international conference is to move, construct, and interface with logical phases where a diverse group of analysts, researchers, academics, and business leaders are hard at work constructing and creating society. I extend my heartfelt congratulations and best wishes for the success of the meeting.



Professor T. S Pillay

Professor of Chemical Pathology, University of Pretoria, Pretoria (South Africa)

from gathering who had made a dynamic, adaptable, inventive and specialized stage for us all. I'm glad to serve this global gathering. I'm certain that the general get-together, which will occur on May fifteenth and sixteenth, will be astonishing and will help in the recreation of our charming society by supporting normal living proclivities. The objective of this worldwide gathering is to move, develop, and interface with legitimate stages where an assorted gathering of examiners, specialists, scholastics, and business pioneers are working diligently building and making society. I broaden my sincere congrats and all the best for the accomplishment of the conference.



Prof. Sangeeta Shukla

Vice-Chancellor, University, Gwalior M.P. (India)

I would want to convey my gratitude and my respects to all of the conference's elite members for creating a lively, flexible, inventive, and technical platform for us all. I am honored to be a part of this conference.

I'm convinced that the overall event, which will take place on May 15th and 16th, will be fantastic and will contribute to the re-establishment of our pleasant society by encouraging common life habits. This international conference aims to move, develop, and interface with logical phases in which a broad mix of analysts, researchers, academics, and business executives are hard at work developing and developing society. I'd want to express my deepest congrats and best wishes to all members of this international conference.

ABSTRACTS accepted in

The 2nd HeriCure-Ukzn: A Hybrid International Conference and Webinar

on

"Recent Progress in Bioactive Compounds & Molecules against Respiratory Diseases and Comorbidities: Theranostics and Future Challenges"





ON

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Pune, India, May 15-16, 2021; Time: 16:30 PM to 20:30 PM (IST) UTC/GMT

IL -1

Peptides, Key Building Blocks for Drug Development

Fernando Albericio, Beatriz G. de la Torre

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Peptides have experienced a remarkable renaissance as therapeutic agents in recent years. They are situated between small molecules (<1000 Da) and proteins, two of the most extensive classes of well-established therapeutic agents.

Peptides provide both the specificity and potency of larger protein biologics but with zero or low immunogenicity. Furthermore, they are smaller, more accessible and cheaper to manufacture using chemical methods, thus presumably combining the advantages of the two therapeutic approaches. While nature has been fine-tuning the bioactive chemical structure of these structures for thousands of years, peptide chemists and protein engineers have the exciting challenge of improving the intrinsically unfavorable pharmacokinetic properties of the majority of native peptides. The drawbacks of peptides as therapeutic agents are associated with their generally high conformational instability.

In this presentation, we will review one example of our research devoted to the synthesis of natural cyclic peptide targeting cancer.

Keywords: cancer, natural products, peptide, solid-phase peptide synthesis





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ON

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Single domain antibodies (nanobodies), the Ninjas of the immune system applications in Covid19

Tahir Pillay

Department of Chemical Pathology, University of Pretoria, South Africa

The control of the Covid-19 pandemic requires convenient and affordable access to testing and diagnosis. Nucleic acid testing has diagnostic accuracy but this usually requires a laboratory, trained personnel and closed proprietary systems hampering access and throughput in a reasonable amount of time. Rapid antibody testing has assisted in mapping the spread of the disease but not in immediate diagnosis. Alternative diagnostic approaches using isothermal amplification of viral nucleic acid and rapid antigen tests to detect viral protein have been used. Rapid antigen tests are advantageous as they are fast, potentially more affordable and available for use with minimal training. One approach we have taken is to use nanobodies directed against SARS-CoV2 to develop both biosensors and rapid lateral flow immunoassays that work on saliva rather than the uncomfortable nasopharyngeal swabs. Nanobodies have the potential to revolutionise diagnostic testing because of temperature stability and robustness for gene manipulation and alteration in the laboratory and low production costs. Nanobody-based assays can be used to complement nucleic acid and serology testing and also identify reservoirs of the virus, to prevent subsequent waves of infection.

Apart from diagnosis, antibodies directed against the major SARS-COV2 proteins (eg. spike) have the potential to be used in therapy either by injection or inhalation. In the most famous example, President Trump received 8 g of monoclonal antibody for treatment. Currently, there are several conventional monoclonal antibodies that are licensed for use in Covid-19 (Eli Lilly and Regeneron) but these are expensive to produce limiting worldwide availability. Nanobodies can replace conventional monoclonal antibodies for therapy. We have produced nanobodies that neutralize viral replication up to 100% in a pseudoviral neutralization assay. Nanobodies therefore provide a bridge between vaccine availability and uptake and will be an important tool in the Covid-19 armamentarium.





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IL -3

Use of Theranostic Pair of Radionuclides in the management of Cancer

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SO/G

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Theranostic pairs of radiopharmaceuticals intended for use in diagnosis and treatment of cancer have been developed at RMC and is being used routinely in patients. Gallium-68- and Lutetium-177-labeled DOTA-TATE constitute a theranostic pair and are used for diagnosis and therapy of neuroendocrine tumor. DOTATAE labelled with Gallium (Ga-68), a positron emitting radioisotope sourced from ⁶⁸Ge/⁶⁸Ga Generator, is a somatostatin-2 receptor analog and is an ideal candidate for imaging neuroendocrine tumors. Indigenous produced [Lu-177] LuCl₃ procured from BARC/BRIT, is used to formulate ¹⁷⁷Lu-DOTATAE and has affinity for Somatostatin 2 receptor in the neuroendocrine tumors. The beta energy (four beta groups 497keVβmax) emitted during the decay of ¹⁷⁷Lu helps in killing of the tumor cells and accompanying 208KeV gamma photons assists in dosimetry and diagnostic evaluation. Similarly, Gallium-68- and Lutetium-177-DOTA-PSMA constitute theranostic pairs and is used for prostate cancer management. Recently use of Yitrium-90 having 2.28MeV BMax suitable for large tumors and Ac-225 a emitter suitable for single cell or small cluster of cancer cell are emerging as potential partner for theranostic pair. At RMC radioisotopes is being used in diagnosis of several pathology involving lungs and respiratory diseases. Theranostic pair of radioisotopes can be extrapolated to other cancers including respiratory diseases provided a suitable target specific ligand is available.





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IL - 4

Exploring aminoglycosides resistant *Mycobacterium tuberculosis* isolates through proteomics and its implications

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Tuberculosis (TB) is one of the most lethal infection among infectious diseases. Mycobacterium tuberculosis, the causative pathogen, causes significant mortality and morbidity worldwide. Drug-resistant TB continues to be a public health crisis. Increment in multidrug-resistant tuberculosis cases (MDR-TB) and its recurrence has driven an increased interest in understanding the mechanism of drug resistance. Aminoglycosides drugsstreptomycin, kanamycin and amikacin are broad spectrum antibiotics and are important antimycobacterial drugs for category-II patients. Molecular studies have indicated various mechanisms for resistance. However, in one third of the resistant isolates no mutation was found. Proteins being the functional moiety of a cell, manifest most of the biological processes and hence are attractive targets for developing drugs, diagnosis, or therapeutics. Completion of the genome sequence along with technological achievements has paved the way for proteome analysis of mycobacteria. Keeping in mind the above facts, we performed proteomic analysis of aminoglycosides susceptible and resistant isolates by two-dimensional gel electrophoresis and their identification by mass spectrometry and bioinformatics. We found few overexpressed proteins in resistant isolates which were either hypothetical proteins or proteins with unknown functions In silico docking analysis showed significant interactions of aminoglycosides drugs with hypothetical proteins which clearly indicated a well-defined cavity on their surface for the binding of drugs. As the initial findings indicate the probable role of hypothetical proteins in aminoglycosides resistance, functional and clinical relevance of these proteins becomes necessary. It is hypothesized that development of simple diagnostic biomarker could rapidly detect early resistance and therefore underlying disease. Structural and biophysical characterization can pave the way to identify drug target molecules.





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IL - 5

Use of immunomodulators as an adjunct therapy in tuberculosis

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Tuberculosis, caused by *Mycobacterium tuberculosis* (MTB), is one among the major leading cause of mortality globally. In 2019, an estimated 10 million people fell ill with TB and a total of 1.4 million people died from TB worldwide of which 0.45 million are from India. About one-third of the world population is infected with *M. tuberculosis* but, interestingly only 10% of it have risk of developing the disease at some point in their lives. The severity of the infection and its outcome depends on a complex interplay between the host and the pathogen and their genetic makeup. The innate immune responses to MTB by macrophages play a crucial role in the host defense and may contribute to variations in immunopathology. Our laboratory is involved in studies to understand the host's response to different lineages of human-adapted MTB and interesting results have been observed which would be discussed. The emergence of Multi-drug resistance (MDR) TB, extensively drug-resistant (XDR) TB and HIV co-infection have exacerbated the global scenario of the disease. The developments of new drugs that can act against MDR and XDR TB and/or the one that will shorten the chemotherapy are the priority in TB research. Worldwide, there is an expanding interest in plant derived products for their anti-microbial activity. A study for screening of various plants derived products for their anti-TB activity was initiated in our laboratory. Further, it is now clear that in absence of the effective immune response, anti-TB drugs cannot eliminate the TB bacilli completely. Thus, to boost the immune system itself, the use of compounds with immunomodulatory activities along with the chemotherapy is a novel approach emerging for the treatment of TB. this approach are that it can kill organisms harbored intracellularly, The advantages of generate protective memory responses and is impervious to the emergence of drug resistance by tubercle bacilli. Immunomodulators proved to be effective as an adjunct therapy will be discussed.

Keywords: tuberculosis, immunomodulator, plant product.





ON

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IL - 6

Second wave of Coronavirus in India: What makes mutated stain of SARS-CoV-2 to become more virulent and pathogenic?

Dhruv Kumar

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The second wave of coronavirus has created health disaster in India and thousands of people have lost their lives. The genome sequencing of over 15,000 COVID-19 cases of Indian patients, revealed a new variant with two new mutations which may be better at evading the immune system. In 15-20 per cent of samples from Maharashtra a new, double mutation in key areas of the virus has been detected. These two mutations are E484Q and L452R mutations. Whereas, other mutations, D614G, L37F, P10S, P13L, A97V, T1198K etc. are also detected in patients' samples. These mutations are important because they are located in a spike protein, that is the region coronavirus uses to penetrate human cells. The spike proteins interaction happens with human cells through a "receptor binding domain", called the angiotensin converting enzyme 2, or ACE2 "receptor," ACE2 protein provides the entry point for the coronavirus to hook into and infect a human cell. These new mutations include changes to the spike protein that make it a "better fit" for human cells. This means the virus can gain entry more easily and multiply faster. It has been hypothesized that these mutations might also make it harder for our immune system to recognize the virus due to its slightly different shape. Therefore, our immune system may not be able to recognize the virus to control the infection through producing antibodies against it. Thus, identification/repurposing of potential inhibitor against specific mutated strain could help us to control the infection and propagation of mutated stain in humans.

Keywords: SARS-CoV-2, Mutation, Coronavirus, Drug repurposing





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IL - 7

Sulfonimidamide: A Less Explored but Potential Scaffold for Synthetic and Bio-applications

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Sulfonimidamides (SIAs), the mono aza-analogues of sulfonamides (SAs), in which one of the sulfonamide O-atom has been replaced by a *N*-atom, were first published by Levchenko et al. in the early 1960's. But the chemistry and applications of these hexavalent stereogenic sulfur moities were long been overshadowed. However, during the last two decades, there has been an increased attention in this functional group in the areas of synthetic- and biological chemistry, as well as material science. As part of our ongoing research work on the preparation and synthetic applications of sulfonimidamides (SIAs), we have developed few new methodologies for the synthesis of various types of SIA derivatives via efficient conditions.





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IL - 8

Phage Derived Proteins for Gram Negative MDR Pathogens: A Potential Alternative

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Bacteriologically confirmed treatment failures are now widely reported owing to an increase in resistance to numerous drug classes, including commonly used β -lactams, macrolides and fluoroquinolones. Hospital acquired gram negative infections are a major challenge to patient safety. Studies have shown that 50-70% of all UTIs are caused by MDR organisms so there is urgent need to have alternative therapy. Bacteriophages (viruses of bacteria) are unique class of naturally evolved recognition probes for bacteria. They are highly host specific and can recognize only bacteria of one species or only one particular strain. Phages, which are major predators of bacteria in nature, were viewed as potential antibacterial agents decades before the clinical development of antibiotics. Being ubiquitous in all natural environments, it is possible to isolate bacteriophage against any of target bacteria. They are highly specific to bacterial host and are stable in wide range of environmental conditions. Thus, presents as a unique class of naturally evolved recognition probes for bacteria as well as therapeutic alternative to standard antibiotic treatment. Also, combination of more than one phage, a Phage cocktail is being reported to have broad spectrum activity against many common pathogenic bacteria. Before selection for its therapeutic role, the phages are characterized by isolation of potential lytic phages, physical and in-vitro characterization in multiple steps, cocktail preparation and purification, dosing and in vivo studies. Endolysins are phage-encoded hydrolytic proteins which acts on peptidoglycan layer and bring about rapid lysis and death of the bacterial cell when applied as purified recombinant protein to bacteria.

Keywords: Phage lysin, Peptidoglycan hydrolases, Gram negative bacteria, Antimicrobial resistance, MDR, Biomedical applications





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UNMASKING MUCORMYCOSIS

Humeera Mulla

Aditya Birla Hospital Memorial Hospital, India

Mucormycosis is an angioinvasive saprophytic fungal infection that belongs to the class of phycomycetes of the order Mucorales. It is the third invasive mycosis in order of importance after candidiasis and aspergillosis. It usually occurs in immunocompromised patients but can infect healthy individuals as well. The predisposing factors for mucormycosis are uncontrolled diabetes (particularly in patients having ketoacidosis), malignancies such as lymphomas and leukemia's, renal failure, organ transplant, long term corticosteroid and immunosuppressive therapy, cirrhosis, burns, protein energy malnutrition and AIDS.

This microbe may be cultured from the oral cavity, nasal passages, throat and stool of healthy patients without clinical signs of infection. This fungal infection usually originates from the paranasal sinuses. The fungus invades the blood vessels and subsequently spreads through them. Once fungal hyphae enter into the blood stream they can disseminate to other organs such as cerebrum or lungs which can be fatal for the patient. Mucor hyphae form thrombi within the blood vessels that reduce vascularity to the tissues and cause necrosis.

Rapid diagnosis and initiation of therapy is critical due to the acute, fulminate nature of the infection. Diagnosis of mucormycosis rests upon the presence of predisposing conditions, signs and symptoms of disease, observation of fungal elements of specific morphology in histological sections, and direct smears of material, and, to a lesser extent, culture result. Thus, early diagnosis can lead to prompt treatment and better prognosis.





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IL - 10

Agnihotra – Healing our environment as a precaution against disease

Ulrich Berk

Environmental Pollution is now one major cause of diseases and deaths worldwide. Never before in known history have we seen such a terrible destruction of Nature, of our Mother Earth. The air we breathe is toxic, the water in our rivers is no longer safe to drink, and the soil is getting depleted at an alarming rate.

Corona also shows higher infection rates and higher morbidity in polluted areas.

In this situation it seems plausible to make use of every method including traditional knowledge which may help to overcome these problems (as it was suggested in the Convention on Biological Diversity (known also as the Rio Convention).

Homa Therapy with Agnihotra (a healing pyramid fire attuned to the biorhythm of sunrise and sunset) as its basic tool comes from ancient Vedic Knowledge and has wide-reaching beneficial effects on our whole environment, means on our atmosphere, on the soil, and on our water resources. Bacteria in air are reduced, water purified, and beneficial bacteria in soil prosper whereas harmful microbes are controlled.

For the present situation of Covid-19, Agnihotra helps in three different ways:

1. Reducing the probability of getting infected.

2. Reducing preexisting conditions (like asthma or tuberculosis) thus

leading to a less severe course of Covid-19.

3. Supporting the body to overcome the Infection especially by reducing stress and strengthening the immune system.





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ON

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COVID-19 prevalence in lung cancer subtypes: Therapeutic Opportunities and Challenges

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¹Department of Biosciences, Manipal University Jaipur, Rajasthan, India

Millions of people are being affected with the novel coronavirus disease (COVID-19), caused by severe acute respiratory syndrome coronavirus type 2 (SARS-CoV-2) around the globe. Cancer patients along with COVID-19 present unique and unfortunate lethal combination with lung cancer patients remain at a higher risk to SARS-CoV-2 infection and its related severe outcomes. To predict the severity of COVID-19 disease in lung cancer patients understanding of underlying molecular mechanisms is become very critical and pivotal. To understand molecular mechanism, we analyzed bioinformatics dataset to analyze ACE2 receptor expression (Gateway of SARS-CoV-2) by using TIMER database. Our study showed promising correlation between immune-modulators and virus receptor proteins certainly, shed light on immunomodulatory therapies to overpower the deregulated pro-inflammatory action in COVID-19. Overall, our study shed a light on differential vulnerability and complications toward SARS-CoV-2 infection in lung cancer types, necessitating a comprehensive and multidisciplinary treatment approach for better outcome during the current pandemic.





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IL - 12

The impact of ACE-2 and associated receptor genes on SARS-CoV-2 infectivity

Theolan Adimulam¹, Dr. Thilona Arumugam¹, Dr. Louansha Nandllal¹ and Dr. Veron Ramsuran^{*1}

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The viral disease, severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) also referred to as COVID-19 (coronavirus disease 2019), has infected more than 155 million people and lead to the death of 3.2 million individuals. The severity of the disease is diverse from one individual to the next. Certain individuals infected with the virus have very mild or no symptoms, while others suffer with serve symptoms, which eventually leads to death. Examining the human genetic contribution to SARS-CoV-2 disease will provide a clearer understanding to varying levels of disease severity. In this study, we examined the human genes that serve as viral receptors i.e. ACE-2, TMPRSS2, BSG (CD147) and NRP1. Studies in the US and Europe have highlighted gender and ethnic differences with respect to death and COVID-19. However, the COVID-19 pandemic has not been characterized from a South African perspective. By comparing the mRNA expression levels of these genes across COVID-19 infected and negative individuals, we observed significant levels of differences for ACE-2, TMPRSS2 and NRP1 (p=0.02, 0.04 and 0.006 respectively). This suggests that host genetic factors are major contributors to the risk of COVID-19 infection, and consequently the extent of disease outcomes. By developing a COVID-19 disease severity profile based on host genetic factors, we will be better equipped to manage future outbreaks and provide targeted therapeutic interventions.

Keywords: ACE-2, BSG, COVID-19, SARS-CoV-2, TMPRSS2





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IL - 13

Small Molecules vs Exosomes: Controlling Cell to Cell Communication

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A new class of picolinohydrazide analogues (5-7) was synthesized via the one-pot reaction between fusaric acid (1) and aryl hydrazines (2-4) using amide coupling reagents. The synthesized compounds (5-7) were characterized using Density-functional theory (DFT) computational spectroscopy besides instrumental methods. Global and local reactivity descriptors of these compounds were calculated at the B3LYP/6-311++g(d) level of theory to predict the reactivity and the reactive sites. The evaluated electronic properties (HOMO and LUMO) gave an insight into the molecular properties of the molecule. The charge distribution and molecular electrostatic potential facilitated the prediction of either the electrophilic or nucleophilic reactivity of these compounds. Extracellular heat shock protein-90 (HSP90) plays an essential role in tumor invasion while epidermal growth factor receptor (EGFR) is found at high levels on the surface of metastatic tumor. Blocking EGFR and HSP90 may predicting metastatic spread. Molecular docking and molecular dynamics showed that picolinohydrazide analogues (5-7) act as inhibitors to the active-site cavity of the target proteins, EGFR and HSP90. The fluorine scaffold (6) has a potential binding free energy of -31.01 kcal mol-1 and -30.54 kcal mol-1 for EGFR and HSP90, respectively. The binding complex of fluorine scaffold (6) with EGFR and HSP90, respectively has also shown substantial stability in the post-dynamics analysis. Our results implicate the potential efficacy of novel adjunct therapeutic insights in treating the advanced cancer.

Keywords: Exosomes, Small Molecules, Inhibitor, Cancer





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Peptide Inhibitors for SARS and SARS CoV2: Current status

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Development of novel SARS-CoV-2 inhibitors is a need of hour. In this regard, here we review some of the peptide inhibitors targeted towards SARS and SARS-CoV-2. Both viruses share similar mechanisms of cell entry involving the viral spike protein. Peptides have been designed and tested to inhibit different stages of the viral entry:

- a) Binding of spike protein receptor binding domain to human ACE2 receptor: e.g., ACE2 binding peptides. However, there is a lack of reports of peptides effectively blocking spike protein- ACE2 interaction and preventing viral entry.
- b) Inhibiting viral fusion with host membrane: After binding ACE2 receptor and thereafter TMPRSS2 cleavage, the spike protein trimer anchors into host membrane and undergoes a huge conformational change forming a six-helix bundle with its HR1 and HR2 domains that helps in fusion of the viral membrane and host membrane. Most of the promising peptides against SARS and SARS-CoV-2 are HR2 based that target HR1 domain and inhibit formation of the six-helix bundle. Xia *et. al.* reported lead peptides based on HR2 domain of SARS-CoV-2 as well as a peptide EK1 based on HR2 domain of HCoV-OC43. Xia *et. al.* later modified EK1 with cholesterol and PEG linker to synthesize EK1C4 which showed 250 times more potency than EK1. de Vries *et. al.* in a separate report, designed an intranasal dimeric peptide based on HR2 domain of SARS-CoV-2 conjugated with cholesterol and PEG linker that prevented SARS-CoV-2 transmission in ferrets.
- c) Prevention of viral RNA release by virus binding and interfering with endosomal acidification: e.g., Peptides P9 and P9R based on mouse beta defensins as reported by Zhao *et. al.*

Keywords: SARS-CoV-2 peptide inhibitor, spike protein inhibitor, viral fusion inhibitor.





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IL - 15

Cordycep militaris: A miraculous fungi having therapeutic potential against emerging diseases

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Medicinal mushrooms have been recognized for thousands of years to produce biometabolites that are used or explored as potential remedies for a variety of diseases. Mushrooms may be possible to deter or reduce nearly two-thirds of cancer-related deaths by containing antioxidants. Cordyceps sp. is a medicinal fungus having important pharmacological and therapeutic implications, particularly for human health, making it an excellent candidate for traditional medicinal use. Different types of necessary amino acids, vitamins including B1, B2, B12, and K, different forms of carbohydrates including monosaccharides, oligosaccharides, and many medicinally significant polysaccharides, proteins, sterols, nucleosides, and other trace elements can all be found in Cordyceps. Cordyceps sp. has been reported to contain a number of bioactive compounds (Cordycepin). Cordycepin has gotten a lot of attention in the past due to its broad-spectrum biological activity, according to prior studies. Purine biosynthesis, DNA/RNA synthesis, and mTOR (mammalian target of rapamycin) signalling cascade are among the biochemical and molecular processes that it is known to disrupt. Cordycepin, a new bio-metabolite with powerful anti-cancer, anti-oxidant, and antiinflammatory properties, is the main ingredient of the extract obtained from this fungus. Cordyceps is a natural medicinal mushroom that is popular among individuals these days, who choose natural medicine over chemotherapy due to the lower risk of negative effects. To develop *Cordyceps militaris* for mass-scale manufacturing, its growth properties must be investigated in depth so that enough bio-metabolites can be extracted from its mycelium fraction. The need to extract and increase the bioactivity of the metabolites from this entomopathogenic fungus using integrative biotechnological and chemical methods is considerable against emerging diseases.

Keywords: Cordycep militaris, Cordycepin, Biometabolites, Mushroom.





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P - 1

Carbon Content Analysis of Virulent Protein of SARS-Cov-2

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Proteins are essential macromolecules present with in cells and are the primary source of physiological function in all biological systems. They are organic compounds vital for carrying out various biochemical processes, cell signalling, cell adhesion, cell cycle, and metabolism of complex molecules such as carbohydrates, lipids and fats to name a few. The primary sequence of proteins is made up of 20 amino acids linked together by peptide bonds. These amino acids are present in numerous combinations in different proteins. The difference in proteins and their function can thus be attributed to these various sequential combinations of amino acids. Proteins sequence analysis at residual level helps in finding sequence similarities, hydropathy profiles, motifs, protein families and specific domains. By going one step further down to atomic level, much extensive analysis of the peptide sequences can be done. The amino acid atoms composition of proteins signifies the basic level of biological organization. The key elements in all amino acids are hydrogen, carbon, oxygen, nitrogen and sulphur. These elements are responsible for giving the amino acids the properties of hydrophobicity/hydrophilicity which play an important role in protein interactions. The hydrophobic amino acids characteristically have greater number of carbon atoms as carbon is the main element which contributes to hydrophobic interactions in proteins. On the basis of hydrophobic/hydrophilic properties of the side chains, each amino acid is assigned a hydropathy index. The higher the index more hydrophobic the amino acid is. The presence of carbon contributes to a higher hydropathy index. Thus, the overall distribution of carbon in a protein contributes to its hydrophobicity. In the current work, the authors have tried to analyze peptide sequences at atomic level taking mainly carbon atoms into consideration. Severe acute respiratory syndrome (SARS) is a newly infectious disease mainly caused by a novel coronavirus, SARS-CoV-2. the SARS-CoV-2 spike protein are composed of two subunits the S1 unit and ither one is S2 unit. The S1 unit contains a receptor binding domain that engages with the host cell receptor angiotensin- converting enzyme 2 and the othreone S2 subunit mediates fusion between the chiral host cell membrane, the S protein play an important key role in induction of neutralizing – antibody and T- cell responses. As well as it works for the protective immunity during the infections of the corona virus. The analysis of all the spike protein of the SARS-Cov-2 and its closely related strain of the corona virus like BAT, MERS and other strain. we can done with the analysis of the strain of the corona virus and check the Carbon, Nitrogen, Oxygen, Hydrogen and Sulphur percentage in the Spike Proteins of the different strains of the SARS-CoV-2. Spike 2003 also a strain of the 2003 corona virus. The carbon content in those spike protein lies between the 32.2-32.1 and hydrogen percentage between the 49.5-49.4, nitrogen content percentage 8.4-8.3, Oxygen percentage 9.6-9.3 and





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sulphur content in the all spike protein lies between the 0.30-0.27. that means a protein of any strain of corona virus having this much of carbon percentage in it. it will work like a spike protein and show virulency on that virus or disease. So, we can say that nature is fixing all the basic atomic level percentage in all spike protein with the different strain of the SARS-CoV-2 which lies between the 32.1-32.2. With the help of the carbon content analysis, we can easily know which protein how much carbon content show the virulency (to cause disease) on that virus or protein in the future.

Keywords: Carbon, COVID19, Protein, Sequence Analysis.





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P - 2

Natural Compounds for the Therapeutic Management of Lung Cancer

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Lung cancer is the leading cause of cancer-related death worldwide. According to the GLOBACON (2018), lung cancer affected about 2.1 million persons (i.e., 11.6% of all cancers) and caused 1.8 million deaths (which comprised 18.4% of all cancer-related deaths). In lung cancer, metastasis has been found to be the foremost reason of mortality (around 90%), and around 70% patients manifest local lymph node metastasis or primary cancer spread at the time of first diagnosis. Therefore, most patients are not appropriate for surgical procedures at the time of diagnosis thereby making chemo- and radio-therapy as main treatment modalities. However, problems like drug toxicity and early recurrence exists with all the present therapies, thereby invoking researchers to find new therapeutic approaches. Recent advances have empowered the biologists for the effective use of natural compounds for the treatment of various cancers. Studies have found that natural products show anticancer effects in numerous ways including inhibition of proliferation, impairment of migration and invasion, shielding lung tissue against carcinogens like cigarette smoke, and augmenting the effects of chemotherapy. Hence, we propose the potential of dietary natural compounds and their bioactive constituent for the prevention and therapeutic management of lung cancer.

Keywords: Lung Cancer, Metastasis, Migration, Natural Compounds, Proliferation.





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Novel 5-methylisoxazole derivatives showing antibacterial, antifungal and antimalarial activity, against the STD drugs

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The present disclosure of the invention presents a novel 5-methylisoxazole derivative & method of preparation thereof. These newly synthesized compounds were characterization and confirmation by LCMS and ¹H-NMR Spectroscopy. These 5-methylisoxazole derivatives showing antibacterial, antifungal and antimalarial activity, against the STD drugs. These compounds would be of better use in drug development to combat bacterial infections and as anti-malarial agents.

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P - 4

Effects of *Ocimum sanctum* L. plant extracts on prostate enlargement

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Prostate enlargement or Benign prostatic hyperplasia (BPH) is a common urological disorder of aging males, which is caused by uncontrolled proliferation of stromal and epithelial cells in periurithral zone of prostate. Ocimum sanctum L. has been used in folklore for the treatment of a wide range of diseases, including urological disorders and known to possess antitumor, antiinflammatory and hepatoprotective efficacy. Therefore, the present study was designed to investigate the effectiveness of the aqueous leave extract of Ocimum sanctum L. (ALEOS) in the BPH rat model. The male rats were treated either corn oil or testosterone (10 mg/kg) dissolved in corn oil and testosterone with ALEOS (100 and 500 mg/kg) consecutively for twenty-one days. The effect of ALEOS on BPH progression was illustrated by prostate weight, prostatic index, percentage of inhibition and histological examinations. ALEOS caused significant reduction in the prostate weight and prostatic index compared to testosterone induced BPH model group. Serum ALT and creatinine levels did not differ among different experimental groups, when compared with a positive control group. ALEOS treated group also ameliorated the hyperplasia of prostate epithelium in a similar manner as observed in the finasteride (5 mg/kg) treated group. This study indicates that ALEOS significantly reduced the progression of BPH and it may be another phytotherapeutial source of drugs in BPH treatment.

Key words: BPH, leave extract, prostate and testosterone.





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P - 5

Design and Synthesis of Tryptophan containing Peptides as Potential

Analgesic and Anti-inflammatory Agents

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A new series of smaller peptides with tryptophan at C-terminal and varying N-protected amino acids/peptides were designed, synthesized and characterized by analytical and spectroscopic techniques. Analgesic and anti-inflammatory properties of these peptides were carried out in vivo using tail-flick method and carrageenan-induced paw edema method, respectively, at different doses and different time intervals. Most of the peptides synthesized displayed enhanced activity, and particularly tetra and hexapeptides 29–31 was found to be even more potent than the reference standards used. Moreover, some peptides have exhibited promising activity even after 24 h of administration, whereas the reference standards were active only up to 3 h. Further, the compounds did not present any ulcerogenic liability.





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P - 6

Recent advancement in the development of bioactive respiratory drugs and COVID-19

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Abstract: Analysis from 1996 to present showed that 180 drug candidates were screened for the treatment of respiratory disease COVID-19.



Figure1: Life cycle of COVID-19 virus. The above diagram (**Figure 1**) clearly indicates that RNA viruses replicates RNA in the human cell. During this process they synthesize their proteins for viral





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envelope which are toxic to human cells. The strategy will be used to develop drug for the treatment of COVID-19 are based on targets in the life cycle of virus. Most of the drugs for the treatment of COVID-19 are repurposed drugs and their modifications.



Figure 2: Targets for COVID 19 and chemotherapeutic antiviral under clinical trials for COVID 19



Figure 3: Future Modification of Remdesivir molecule to get better bioactive molecule for respiratory diseases.

Remdesivir belongs to developed by Gilead Sciences a class of antiviral drugs that inhibit RNA-dependent RNA polymerase, an enzyme essential for some RNA viruses resembling SARS-CoV-2 to replicate. Thus, inhibiting the enzyme might prevent viral replication in





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infected cells. The synthetic protocol for the remdesivier is shown in the (Figure 3) above.

In **Figure 2** various targets for the development of drugs and existing drugs are mentioned. There are huge number of bioactive molecules which can be screened for the respiratory disease like COVID-19. Most of the drugs are chiral therefore the plan should be in such a way to develop chiral catalyst for these drugs².



Figure-4. Bioactive molecules for respiratory infections

Above diagram shows that there are some existing bioactive drug molecules (1-9) used as antiviral and respiratory infections. These are starting molecules whose isosters would be designed and screened for respiratory diseases¹.

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Bioactive compounds in Bamboo shoots and their health benefits

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Foods consumed by us have, besides their basic nutrients, several active ingredients termed as bioactive compounds which impart our food with the means necessary to maintain or even improve our health. Foods particularly rich in such bioactive compounds play an active role in prevention and cure of chronic diseases and are often termed as the functional foods. Diets having optimum proportion of such functional foods will not only help in improving health profiles of consumers but also help in cutting the costs to health care systems prevalent across the world thereby bringing social and economic gains. This fact has brought about an enormous interest in identifying new sources of such functional foods that can contribute to improve our health and well-being. Bamboo shoots, the young, aerial outgrowths of the bamboo plant, have slowly but steadily established itself as a novel functional food with tremendous health benefits. Even though their use as a seasonal delicacy and further applications in traditional medicinal system has been known for centuries across the Asia, it is only very recently that the presence of several bioactive compounds such as phytosterols, phenols and dietary fiber in them has been confirmed scientifically. These bioactive compounds have been proven to impart bamboo shoots with several health benefits such as improvement of bowl function and digestion, reducing serum cholesterol, neuroprotective, utilized inflammatory, antibacterial, antimicrobial and antioxidant properties, prevention of diabetes, obesity, metabolic disorders, cardiovascular diseases and even certain types of cancers. Therefore, with a plethora of bioactive compounds and associated health benefits, bamboo shoots represent an ideal functional food resource which if utilized to its full potential can prove to be a major ally in our quest for a healthy future.





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Plant based antimicrobial peptides as therapeutics

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The role of plant derived compounds has been inevitable in pharmaceutical sciences to exhibit a vital role in sustaining human health. Till date, usage of medicinal plants and their extracts continue to relieve people from illnesses. However, escalating biotechnological epoch pushes the researchers to explore novel antimicrobial drugs against hazardous pathogens infecting humans, more so in view of recent evidences of the increasing predominance of multiple drugs/antibiotics-resistant microbes. In this context, emergence of plant-based anti-microbial peptides (AMPs) as novel and potential antibiotic alternatives has drawn much attention towards their therapeutic use in human healthcare against various Gram-positive and Gramnegative bacterial infections. The AMPs belong to a diverse group of natural bioactive molecules isolated from different parts of the plants, namely roots, seeds, flowers, stems, and leaves. These AMPs have length ranging from 10 to 100 amino acid residues, and play an expedient role in host-defence mechanism. The AMPs exert broad-spectrum anti-microbial activities and also exhibit a crucial role as immune modulators, anti-hypertensive molecules, anti-cancer & amp; anti-tumor agents, and anti-infective agents. They are classified into different families like defensins, thionins, hevein-like proteins cyclotides, lipid-transfer proteins, snakins and several others based on the variation in their structure, composition of amino acids, number of disulfide bonds and mechanism of action. In the talk, plant AMPs will be discussed as promising alternatives to conventional antibiotics for curing human diseases.

Keywords: Antimicrobial peptides (AMPs), plant proteins, therapeutics, defensins.





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Potential bioactivity of *Cordyceps militaris* against viability of lung cancer cell line A549

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Cordyceps militaris is an effective medicinal mushroom having reported potential bioactivity against several diseases. In this present study, we have extracted biochemical compounds present in *Cordyceps militaris*, using HPTLC and analyzed and identified by HPLC. The compound was detected as Cordycepin. MTT cell viability assay was performed on A549 (lung cancer cell line). For this, extract having cordycepin, was completely dried firstly and then dissolved in DMSO. A549 cell line was maintained in DMEM with10%FBS, 1% L-glutamine and1% penstrep. 5000 Cells were seeded in each well of 96 well plates; at 60-70% confluency cells were treated with different extracts of *Cordyceps militrais* at various concentrations. Further, plate was read by ELISA plate reader at 570 nm for absorbance density value to determine cell viability. Viable cells were capable to reduce the tetrazolium salt to formazon resulting in blue color whereas dead cells were not able to do so. Fractions of viable cells were calculated and it was found that the extracts of *Cordyceps militaris* having the anti-viable property against human lung cancer cell line A549.

Keywords: Cordyceps militaris, Cordycepin, lung cancer, HPLC, MTT Assay.





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Efficient Production of the Potent Antimicrobial Metabolite "Terrein" From the Fungus Aspergillus terreus

Jyoti Goutam, Ravindra Nath Kharwar, Vinod Kumar Tiwari, Ranjana Singh, and Divakar Sharma

The endophytic fungus *Aspergillus terreus* (JAS-2) derived from *Achyranthes aspera* possesses multiple bioactive metabolites, one of which is terrein, a potent antimicrobial substance. Here we report the improved biosynthesis of terrein in cultures grown in media with a fixed carbon and modified nitrogen source (4% dextrose, 1% casein) for 15 days, after which pure crystals of terrein were obtained in the culture medium. We suggest that our improved method is effective for improving the quantity and quality of terrein produced. Terrein has shown potent antimicrobial activities against various microbes that may lead to its further use to combat antimicrobial resistance which threatens the community worldwide.

Keywords Endophyte, Terrein, Casein, Natural crystals, X-ray crystallography, High performances liquid chromatography (HPLC).





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Mimicking B epitopes of *Mycobacterium leprae* and host: Predictive biomarkers for pathogenesis of type 1 reaction in leprosy

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Mycobacteria are among the few infectious agents both in humans and in experimental animal models, which have been found to augment autoimmune responses. Several Mycobacterial infections including leprosy and tuberculosis are known to evoke autoimmune responses by modulating homeostatic mechanism of the host. In tuberculosis patients, presence of autoantibodies against a variety of self-components has been reported. Similarly, Presence of several autoantibodies which include rheumatoid factor, antinuclear factor, keratin, myelin basic protein (MBP), and myosin have been earlier reported in leprosy patients. Antigenic/molecular mimicry has been suggested as a way to escape detection and destruction of the pathogen by host. The aim of the present study was to detect the role of mimicking epitopes of *M. leprae* and host components in the induction of inflammatory response by means of autoimmune factors. A total of eleven B cell mimicking epitopes (BCE) of protein HSP65 (*M. leprae*) and protein keratin (host) as well as four B cell mimicking epitopes of protein 50S ribosomal protein, lysyl tRNA synthetase (*M. leprae*) and myelin basic protein (host) have been predicted and were synthesized by outsourcing. Humoral responses against these epitopes were investigated in 50 non-reaction (NR), 50 type 1 reaction (T1R) leprosy patients and 20 healthy controls. We observed significantly higher levels of antibodies against 8 mimicking BCE in T1R in comparison to NR leprosy patients. Among the eight mimicking BCE, three BCE of HSP65 (HSP1; p<0.00001, HSP4; p<0.0001, and HSP5; p<0.01) and three BCE of keratin (Ker1; p<0.00001, ker2; p<0.00001 and ker4; p<0.00001), one BCE of MBP with 50S ribosomal protein (MBP50SB1, p<0.03) and one BCE of MBP with lysyl tRNA synthetase (MBPLMB2, p<0.00001) were found to be significantly associated with T1R. In present study, a total of eight mimicking BCE of the protein's keratin and MBP were found to be associated with T1R. It suggests that the mimicking epitopes plays a key role in induction of autoimmune response in leprosy and inflammatory episodes of T1R in leprosy. These molecules/epitopes may be employed as a biomarker to predict the inflammatory episodes of T1R in leprosy.

Keywords: Autoimmunity, B cell epitopes, Keratin, Leprosy, Myelin basic protein.





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Immunomodulatory activity of aqueous extract of {Ocimum sanctum (os)} as a rat model

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Background: Biochemical, haematological and Immunomodulatory effect of *Ocimum sanctum* in rat was studied.

Objective: To evaluate the immunomodulatory effect of Ocimum sanctum as a rat model

Methods: Aqueous extract of *Ocimum sanctum* were administered orally at doses of 100, 200 mg/kg/day for 45 days in *wistar albino* rats. Immunomodulatory effect and biochemical and haematological changes were tested by standard methods.

Results: Aqueous extract of the *Ocimum sanctum* showed increasing antibody production in dose dependent manner. It enhances the production of RBC, WBC and haemoglobin. It dose not affect the biochemical parameters.

Conclusion: An oral administration of the aqueous extract of O. sanctum showed immunomodulatory effect in rat.





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Docking study of phenolic acid compound present in maize plant against tumor causing genes

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Cancer is a major chronic degenerative illness that affects people all over the world. Consumption of whole-grain cereals and their derivative food products has been linked to a lower risk of various cancers in recent years. Pharmaceutical properties can be found in some of these peptides and have biological effects that are beneficial to one's health and help to prevent cancer. Vitamins (A, B, E, and K), minerals (Mg, P, and K), phenolic acids (Diferulic acid, coumaric acid, and syringic acid), carotenoids and flavonoids (anthocyanins), and dietary fibre are all found in corn nutrients and phytochemicals. More scientific evidence is accumulating that daily consumption of whole grain corn reduces the risk of chronic diseases such as cardiovascular disease, type 2 diabetes and cancer. The biological effects of phenolic acids found in pigmented corns on human health, such as anticancer, antimutagenic, anti-inflammatory, and cardiovascular diseases, make them extremely important. CDK8 and cyclin C bind to the mediator complex and control transcription through a variety of mechanisms. In this current In-silco study, we will do docking study of Diferulic acid against CDK8 - Cyclindependent kinase 8 which is potential inhibitor of CDK8 and present in abundant amount in Maize plant.

Keywords: Anthocyanins, CDK8, Diferulic acid, Maize, Tumor.





ON

"Recent Progress in Bioactive Compounds & Molecules against Respiratory Diseases and Comorbidities: Theranostics & Future Challenges"

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Combinatorial implementation of Computational and Informatics to study Bio-active molecules from various biological sources

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Many stages of the drug discovery pipeline have seen improved efficiency that is due to advances in informatics and computational biology. Despite this, drug development has slowed, owing to a heavy dependence on small molecules as a source of new possibilities. Bioactive molecules have been known to have medicinal properties since the dawn of time. Biological sources like plant and its derived medicines, utilized to treat a variety of pathologic conditions. Computer-aided drug discovery/design methods have played a critical role in the creation of therapeutically significant biomolecules. This has resulted in faster drug development and evaluation of candidate compounds' safety, pharmacokinetics, and effectiveness, as well as novel drug design and synthesis methods based on natural compounds. Recent developments in informatics and computational methods have paved the way for new ways to process complex natural products and use their structures to create novel drugs isolated from different biological resources. Structure-based methods are similar to high-throughput screening in that they require both target and ligand structure information. Ligand docking, pharmacophore, and ligand design methods are examples of structure-based approaches. The identification of molecular targets of natural products and their derivatives has been aided by predictive computational tools. Quantum computing, analytical tools, and databases can be used in the future to model molecular interactions and predict features and parameters needed for drug production, such as pharmacokinetics and pharmacodynamics, resulting in less false positive leads in drug development. Bioinformatics approaches for drug discovery include sequence-based features, interactions with body structures metabolites, proteins, cells, tissues, pathway perturbations, and toxicity. It also includes fields such as multi-omics and highthroughput sequencing that play a significant role in analyzing different gene interactions in non-infectious and infectious conditions. Thus, combinatorial implementations had fastened the research domain in terms to find and evaluate natural bioactive compounds through computational and informatics approaches.

Keywords: Bio-active molecules, Drug design, Ligand, Pharmacokinetics, Quantum computing.





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An Investigation of Algal Specimen of the Choral River with Special Reference to Chlorophyceae, at Choral, district Indore, (M.P.)

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The present study was conducted to understand the diversity and distribution pattern of microalgae in freshwater system found in Choral River. A variety of were identified belonging to various texa of Algae during July 2019 to June 2020. The identified of 08 order belonged to Chlorophyceae. The colonial, filamentous, non-filamentous algal Specimen were recorded from sites, in this research study total 16 algal form were observed from three different sites of Choral River. The present study recorded 3 species of order Zygnematales, 2 species of Volvocales, 3 species of Sphaeropleales, 2 species of Chlorococcales, 2 species of Desmidiales, 2 species of Cladophorales, 1 species of Oedogoniales, and 1 species Chaetophorales were recorded. The algal species from freshwater samples collected algal flora is identification and description of from different three sites of River as well as algal diversity was observed under microscope.

Keywords: Algal Specimen, freshwater, diversity, Chlorophyceae, Choral River.





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Capsaicin to combat SARS-CoV-2 receptors: A molecular docking approach

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Main protease (Mpro) theaters a vital role in processing of CoV-encoded polyproteins which facilitate the gathering of replication-transcription tackle and is hence recognized as a perfect antiviral target. In the current work we have performed the docking analysis of the SARS-CoV-2 receptor Nsp9 RNA binding protein (PDB Id: 6W4B), Mpro Replicase polyprotein (PDB Id: 6Y84) and Nsp15 endonuclease (PDB Id: 6VWW) with a number of chemical compounds namely: tinosporin, capsaicin, curcumin and oleuropein. Amongst the all, capsaicin, an alkaloid in nature and the active compound of *Capricum annum* showed the best binding efficiency. Capsaicin has been broadly used for treatment of muscular pain, headaches and many forms of cancer. In this work, molecular docking basically blind docking was performed by Autodock Tools version 4.2 by means of genetic algorithm, to evaluate the estimated free binding energy of the docked compounds. The results were analyzed which revealed that capsaicin displayed best binding energy with Mpro Replicase polyprotein that is -7.03kcal/mol, -5.76kcal/mol energy with Nsp9 Replicase binding protein and -5.36kcal/mol with Nsp15 endonuclease and hence could be presented as a potent molecule against this pandemic. The results could be further refined by rigorous molecular dynamics studies.

Keywords: AutoDock, Capsaicin, Mpro, Nsp9, Nsp 15.





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Coenzyme Consortium of Tyrosinase and Laccase for medical application

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The sequential rise in the atmospheric carbon di oxide concentration due to anthropogenic emission of this gas has resulted in elevation of the average mean global temperature resulting in a drastic effect circumventing to climate change. Biomimetic approach involving carbonic Anhydrase has provided an interesting rationale for sequestration carbon di oxide into calcium carbonate which will be concurrently used for mushroom production. Tyrosinase and Laccase extracted from mushroom purified and then subsequently used for the conversion of phenolic waste from different source to humus. Previous studies on abiotic and biotic catalysis have focused on polyphenols, amino acids and sugars, while no work has been done on lipids, one of the most refractory components of plant materials and a significant contributor to the humin fraction of soil organic matter. Use of advanced analytical instrumentation, i.e., synchrotron-based X-ray absorption spectroscopy, Spectro microscopy and infrared spectroscopy, atomic force microscopy, multi-dimensional nuclear magnetic resonance spectroscopy, and the like should shed light on the mystery of environmental humic substances and their complexes with mineral particles.





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CAR T-Cell: Immunotherapy for Cancer Treatment

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Cancer is a major public health challenge. According to WHO 2020 report, 10 million death of people were listed as cancer. According to current research, scientists have developed a new treatment to overcome this hazardous problem with the help of a special type of therapy which is based on modifying T cells called as Chimeric Antigen Receptor (CAR) T Cell. CAR T- cell therapy is a novel kind of immunotherapy. It is designed to strengthen and harness the immune system inherent cancer eliminating powers by genetically modifying T-cells, a vital part of the immune system. Currently used for the treatment of blood cancers including Acute Lymphoblastic Leukaemia, Transformed Follicular Lymphoma, Primary Mediastinal Large B-Cell Lymphoma and Diffuse Large B-Cell Lymphoma. Traditional immunotherapy attaches drug in patient's T-cell's, destroy cancer. CAR T-cell treatment creates patients own T-cells, engineered lab to re-infused large numbers and destroy cancer cells with no drugs involved. Thousands of patient's own T-cells collected, blood removed from the patient's arm. Amplified. Then millions of CAR T cells are grown and re-infused into the patient. Results for clinical trials using CAR T-Cell Therapy for the treatment of B-cell malignancies, including B-cell Acute Lymphoblastic Leukemia (ALL), Hodgkin and Non-Hodgkin Lymphomas (HL, NHL) have been very promising. The US Food and Drug Administration (FDA) has recently approved the two CAR T Cell Therapies, Tisagenlecleucel (Kymriah) for ALL and Axicabtagene ciloleucel (Yescarta). Early data from this exciting new treatment shows promising results for many patients. HCA Healthcare UK, one of the first JACIE accredited UK private offers CAR T-Cell therapy. CAR-T holds great promise in the treatment of cancer. It is clear that CAR T-cell therapies has given positive hopes in the future of cancer immunotherapy. CAR T-cells are the resurrectors in cancer treatment.

Keywords: Cancer, Immunotherapy, CAR T- Cell, Treatment





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Bioactive compounds and molecules against Covid-19

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Covid-19 Pandemic! Because of which every human being in the world is trampling. This pandemic has affected more than 153 M people and more than 3.2 M people have lost their lives in the world so far. Covid-19 causing virus, Coronavirus (CoVs), is a member of positive sense mRNA family which causes lethal human respiratory illnesses named SARS (severe acute respiratory syndrome). The vaccination had been initiated in many countries including India. The spreading of virus had been controlled in the first wave to a large extent but in the second wave there are some strains of virus which has mutated itself. These mutated strains of virus are spreading very rapidly across the worldwide. Because of the mutated strains of the virus the efficacy of vaccine is also reduced up to a certain extent.

Several researches has shown that bioactive compounds and molecules have physiological, behavioural and immunological effects.

Bioactive compounds and molecules are the nutritional constituents that are found in small quantities in food providing health benefits beyond the basic nutritional value. These are also called secondary metabolites. Some examples are alkaloids, flavonoids, vitamins and minerals, choline, etc. The immunological effects of the bioactive compounds and molecules have been used since decades.

Since there is no confirm treatment and strategies for the pandemic the bioactive compounds and molecules can thus be great help in improving immunity. As it has been found that the affected individuals with high immunity have a high recovery rate.

Keywords: Bioactive compounds, Pandemic, Coronavirus, SARS, Flavonoids.





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Comparison of Antibiotic susceptibility patten of clinical isolates from respiratory tract infection using automation system

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Respiratory tract infections (RTIs) are highly contagious and prevalent, enhances morbidity and mortality to a large population. Special treatment and attention are required if the infectious agent is resistant to the existing antibiotics. Large number of human infections were associated with pneumonia like syndrome during the respiratory illness. This study aims to determine and compare the antibiotic susceptibility pattern of clinical isolates for respiratory tract infection using two automation system viz: BD Mx50 and Vitek 2 compact. A total of 56 samples were collected and processed on both the automation for antibiotics susceptibility assay, out of above, Vitek 2 Compact identify Escherichia coli (30%), Klebsiella pneumonia (28.5%), Pseudomonas aeruginosa (16%), Citrobacter (5.3%), Acinetobacter baumanni (7.2%), Brucella melitensis (1.7%), Providencia rettgeri (5.4%), Salmonella paratyphi (1.7%), Stenotrophomonas (3.5%). While going through susceptibility, we found a different pattern of resistivity by different isolates. In these isolates, 29% of bacteria are extended-spectrum betalactamase (ESBL) producer, 52% isolates were Carbapenemase producers, 3.5% isolates were cephalosporins producers, 3% isolates are quinolones resistant, 9% isolates did not show any findings and 3.5% were consistent. Whereas, BD Mx50 shows that isolates are Escherichia coli (30%), Klebsiella pneumonia (28.5%), Pseudomonas aeruginosa (14%), Pseudomonas pseudoalcagenes (1.7%), Citrobacter koseri (3.5%), Citrobacter farmeri (1.7%), Achromobacter (1.7%), Acinetobacter (5.3%), Stenotrophomonas (2%), Providencia rettgeri (3.5%), Leminorella grimontti (2%), Salmonella (2%), Alcaligenes (2%). BD Mx50 does not identify Brucella. The pattern of antimicrobial susceptibility shows different results. 18% isolates show ESBL production, 4% isolates were Class A Carbapenemase producer, 16% isolates were Class B Carbapenemase producer, 12% were Class D Carbapenemase producer,18% isolates were Carbapenamase producers, 32% isolates did not show any findings. While comparing the time taken by both the automation, BD Mx50 is taking 2 hours more than Vitek 2 Compact. The conclusion of this study is, BD Mx50 is differentiating between classes of Carbapenemase, so we can use it to check multiple drug resistance and Vitek can be used in case of hospitals where more sample load is there. Although, study using





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large sample size will warrant the use of these automation system in finding the resistance pattern more accurately under clinical settings.

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Characteristics Codon Usage Bias in SARS-CoV-2 Virus

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Whenever there is an advent of any new strain of any virus, there is a large set of rearrangements in its respective viral genome. This research work is a preliminary work into unravelling some of these changes. During the process of evolution, the virus has acquired certain unique codon biases which has given an exclusive identity to SARS-CoV-2 i.e., Wuhan Corona Virus. Whilst designing a vaccine for a particular organism and if you are targeting any particular protein or an Open Reading Frame (ORF) which encodes for no- structural protein. Those codons which are very much under-represented, they are going to be preferred over here as compared to those that are over-represented. The analysis of the Wuhan Corona Virus represented that it is closely linked to SARS-CoV-Tor2, SARS-CoV-Urbani and Bat Corona Virus but distantly related to MERS-CoV. Because there are evidences where we see that there are 4 regions of similar to all other four viral genomes than MERS which makes it a distant relative. It has attained this capacity while reaching an equilibrium in the codon usages or highly preferring to certain codons counter to its close neighbours such as SARS-CoV-1 or Bat Corona Virus. Taking into account all the analysis formulated in this study we can say that SARS-CoV-2 has relatively low codon usage bias as compared to other relatives but has a close phylogenetic relationship with Bat Corona Virus. The low codon usage bias might be due to the selection pressure as well as mutations. There are peculiar features inimitable to Wuhan as compared to others. And this data can be exploited for diagnostic or making vaccines not





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forgetting that another huge round of analysis needs to be done afterwards for coming with vaccines that are operative against these viruses.

Keywords: Codon usage pattern, Insilico Analysis, SARS-CoV-2.





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Succession of Chickpea (*Cicer arietinum* L) and their management through biopesticides and fungicides

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Collar rot of chickpea by *Sclerotium rolfsii* (sacc.) is a disease, usually appear at seedling stage under agro condition of Jabalpur, Madhya Pradesh. The pathogen survives in the soil and perpetuate in the form of sclerotium bodies. Influence of 6 fungicides 4 biopesticides and 2 phytoextract employed as seed treatment was determined. Results of investigation indicate that seed treatment with carboxin + Thiram@ 0.03% resulted in minimum seedling mortality (13.4%) and 53.79% diseases control over check with 29.0% seedling mortally at 24 DAS, followed by seed treatment with copper oxychloride 18.0% mortality and 31.03% disease control, Among biopesticides, *Trichoderma harzianum* exhibited 21.2% mortality and 31.03% disease control where Neem leaf extract 26.4% mortality and 8.56% disease control was noticed after 24 DAS under natural held condition.

Keyword: Chickpea, collar rot, Sclerotium rolfsii, Seed treatment.





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Effect of pH and temperature change on survivability of coliphages

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Escherichia coli is one among the foremost studied bacteria within the world and is arguably acting as a model microorganism for research. In humans, E. coli is one of the most frequent causative agents for urinary tract infections, appendicitis, pneumonia, bloodstream infection and gastrointestinal infections. In recent years, E. coli is showing resistance towards Norfloxacin, amoxicillin, gentamicin, cotrimoxazole, Augmentin, Ciprofloxacin, Streptomycin and Nalidixic acid. Antibiotic resistance is one of the toughest challenges faced by doctors and researchers as treatment of patients is very difficult as no antibiotics work. Effective novel approaches for treatment of infections induced by this pathogen are therefore necessary. Phage therapy represents a promising alternative solution to eradicate antibiotic- resistant pathogens. It is also important that the phages have good survivability and storage capacity. High biodiversity of the collection is indicated by its biological characteristics i.e host range, plaque size and morphology, growth at various temperature, thermal inactivation, sensitivity to low and high pH, sensitivity to osmotic stress, etc. In the present work, we have characterised the isolated coliphages for temperature and pH resistance. After the plating of sewage sample, five different types of phage plaques were observed. In physical characterization, isolated bacteriophages revealed significant biological features, like ability to form plaques at low temperature (4°C), resist high temperature (62°C and 95°C) and survive in a wide pH range (4.0-10.0). A survival percentage of 75-95% was seen at pH 10, whereas the range was 40-58% for pH 4.0. Two out of five isolated coliphages had good survivability in presence of organic solvents (ethanol, acetone, DMSO, chloroform) or detergent (SDS, CTAB) making them potentially interesting in the context of biotechnological applications like phage therapy. The two most potential strains will be further characterized by transmission electron microscopic (TEM) analysis and sequencing.

Keywords: Escherichia coli, MDR, Coliphages, Phage therapy, Physical characterization





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Recent Physiotherapy & Herbal compounds progression in SARS-Cov-19 against Cardiorespiratory disease and Comorbidities

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The present global pandemic of Covid-19 has brought the whole world to a standstill, causing, morbidity, death. The common cause of death and morbidity nowadays are pneumonia and respiratory failure. Patients require ventilation and other techniques like cardio-respiratory physiotherapy and its result to exchange the gases and improve lung function. It is also provided with patients early respiratory conditions for Covid-19 cardio-respiratory physiotherapy. The way to help people with cystic fibrosis clear their lungs of thick and sticky mucus that can clog the airway some time huffing coughing is the best way to clear the airway and also a good way to reduce lung infection and improve lung function. The goal of positioning is to drain the mucus from every five lobes of the lungs by draining it. It may be coughed out, percussion/clapping with the hand or percussion clips over the lung segments will loosen the mucus, and coughing will move it out to the larger airway. Even in patients after discharge from the hospital. Cardio-respiratory rehabilitation is one of the forms of training a respiratory muscle, cough exercise, diaphragmatic training, intercostals stretch, and active cycle of breathing technique, apical stretch, percussion, vibration, lung mobilization, dyspnea positioning, forcefully expiratory technique, positive expiratory pressure, prone positioning, and gravity assisted postural drainage, huff, and cough, suctioning pruning is the best positioning for Covid -19 patient to ventilate the lungs. So air can go directly to the lungs all lobes of long. It is contraindicated in pregnant women, people with major cardiac conditions or patients with cardiac surgery, and those with an unstable spine should avoid proning and do not do prone lying position immediately having a meal wait for at least 1-2hrs. Proning is extremely beneficial in covid-19 patients with compromised breathing comfort, especially during home isolation. Incentive spirometry using can help you practice taking deep breaths, which can help open your practice taking deep breaths, which can help open your airways, prevent fluid or mucus from building up in your lungs, and make it easier to breathe.

The Use of Herbal medicines/compounds e.g., Punch tulsi drop, Giloy, Chirata and Mahasudarsan churna to reduce/cure viral (gradually) infection. Antioxidants are naturally present in many fruits so eat too much fruits. To increase the healthy antibody development against viruses.





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Green synthesis and applications of nanoparticles derived from red marine algae of Indian coastal waters; a review

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Few reports in the literature have been reported to synthesize nanoparticles using aqueous extracts of renewable marine algae. It is a least explored research area and has now gained researchers ' interest due to the unique physiochemical properties of nanomaterials, which are responsible for an effective pathway for new pharmaceuticals and medical treatments [1]. This biogenic synthesis is an effortless, modest, and less vital approach; the NP produced by this approach is environmentally friendly [2]. The approach based on green chemistry is nontoxic, because the bioactive chemicals found in marine alga's cell membranes can act as both reducing and capping agents [3]. Thus, there are unique opportunities for exploration and developing new green chemistry based biogenic processes for the production of Silver, Iron Oxide and Zinc Oxide nanoparticles. Over the course of the year, renewable marine resources are available, so researchers are focusing on marine resources such as marine macro algae that are abundantly available along India's coastal areas and across the globe [4]. There are about 841 marine algae known from coastal Indian region [5]. Our current review draws attention to the current progress in the biogenic synthesis of stable nanomaterials, the process of greener synthesis of metal and metallic oxide NPs, from Rhodophytic marine algae from the coastal regions of Indian water along with their size, distribution, morphology and applications such as antimicrobial, antibiofilm, synergistic and anticancer potential are briefly defined and the prospective scope of research.

Keywords: Nanoparticles; Marine Resources; red marine algae; Biosynthesis; Antimicrobial; Antibiofilm; Synergistic; Anticancer; Applications





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Giloy (Amritavalli) and their use for treatment of various infections in human

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Giloy (Tinospora cardifolia) is an important herb that used in medicine. It is also known as Guduchi in Hindi. In Sanskrit giloy is called as amrita it means the root of immortally, giloy also known as shloka of Charak samhita according to Charak. Giloy have bitter taste. Giloy is beneficial in more disorders of body such as immunomodulatory, hepatoprotective, cardio protective, Anti-inflammatory, Antioxidant, Analgesic effects. According to Ayurveda this can be used in different ways, it may be used either in juice form or as powder. Giloy have power to activate immune system, boosting immunity and also fight against different diseases and improve human health. Giloy have antipyretic character which fight against many microbial infections. The stem and leaf of the plants are frequently used in different type fever like dengue, allergic rhinitis, typhoid. Oil extracted from the plant is used as skin lotion and used in skin diseases. Regular use of plant in raw or processed form help production of insulin and thus control blood sugar therefore, the plant is also known as 'Madhunashini' its means destroyer of sugar. Giloy also use in kidney and diabetic ulcer, upgrading digestion problem such as diarrhea, colitis, vomiting, hyperacidic, it contains antiinflammatory and anti- arthritic properties which decrease arthritis problems. Giloy upgrade stronger digestive system and boost immune system against hyperacidity. It is helpful in reducing stress level and anxiety thus regulate physiological functions. This herb is health rejuvenator and successfully intensify natural immune system to fight against more health illnesses.









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