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ICBTM 2024

PROCEEDINGS

3rd International Conference

on

INTEGRATIVE CHEMISTRY, BIOLOGY & TRANSLATIONAL MEDICINE

8-10 March 2024

ORGANIZERS

Hansraj College, University of Delhi, Bharat
Pacific University Udaipur, Rajasthan, Bharat
HeteroChem InnoTech Pvt. Ltd., Bharat

CO-ORGANIZERS

University of Debrecen, Hungary
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Jawaharlal Nehru University, Delhi

Charles University, Czech Republic
Kwazulu-Natal University, South Africa
Kumaun University Nainital
Mayo Clinic Florida, USA
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Mayo Clinic Florida, USA
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Department of BioTechnology, Government of India

ICBTM 2024

Proceedings of

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ICBTM 2024

3rd International Conference
on

INTEGRATIVE CHEMISTRY, BIOLOGY & TRANSLATIONAL MEDICINE

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HANSRAJ COLLEGE

Hansraj College is one of the largest constituent colleges of the University of Delhi. The college was founded by the D.A.V. College Managing Committee on 26th July, 1948 in the sacred memories of Maharshi Dayanand Saraswati and Mahatma Hansraj who spent their magnificent lives emphasizing the importance of knowledge. It is one of the leading lights in the D.A.V. family of over 700 institutions. Hansraj College is a premier institution dedicated to teaching and research. It has highly qualified academicians who impart education in Science, Commerce, and Arts at undergraduate and graduate levels to more than 5000 students. The college has consistently demonstrated outstanding performance in academics, sports, and extracurricular activities.

The college has completed 75 years in the realm of imparting higher education. It has made significant and unparalleled contributions in terms of producing scholars, bureaucrats, intellectuals, and sportsperson serving in different domains not only in our own country but even at international levels.

PACIFIC UNIVERSITY

Established in 1997, the Pacific University has made a mark on the educational map of India. Over the last 25 years, the Pacific Society has continued to make rapid strides in the field of higher & technical education. It has established more than twenty one institutes and become a multi-disciplinary conglomeration of colleges providing higher education in the diverse fields of Engineering, Management & Commerce, Dentistry, Pharmacy, Education, Basic & Applied Sciences, and Research Programmes (Ph.D.) in all relevant disciplines.

Pacific University has a mammoth ultra modern campus sprawling over more than 100 acres of lush greenery, including state of the art classrooms, separate hostels for boys and girls, laboratories, and libraries, internationally benchmarked curricula, innovative pedagogy, experiential learning and affordable quality education, the university is committed to establish itself as a centre of excellence in research.

HETEROCHEM INNOTECH

-A New Era in Drug Discovery

Our Approach

HeCIT is a pre-clinical stage biotech startup with an exciting portfolio of programs. We are committed to pioneering novel therapeutics to treat diseases. HeCIT aims to deliver formidable results by acting in an agile and transparent manner and be recognized for its industry disruptive innovation in healthcare.

To develop a collaborative research platform with a focus on creativity and innovation in science. We aim to provide the best possible infrastructure through combined efforts for rapid advancements in biomedicine.

Life at HeCIT

Here at HeCIT, we believe in an open-minded, friendly, and cheerful work environment. We are working towards the revolution of conventional science through innovation, creativity, and technology. Our team is always inspired to achieve excellence through unbossed leadership.

ABOUT THE CONFERENCE

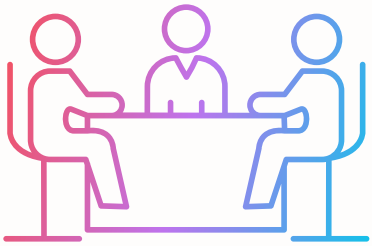
We are delighted to announce the 3rd International Conference on INTEGRATIVE CHEMISTRY, BIOLOGY & TRANSLATIONAL MEDICINE (ICBTM-2024), set to be jointly organized by Hansraj College, University of Delhi; HeteroChem InnoTech, New Delhi and Pacific University, Udaipur, in exemplary partnership with Oswaldo Cruz Foundation (Fiocruz), Recife, Brazil; Charles University, Czech Republic; University of Debrecen, Hungary; Kwazulu-Natal University, South Africa; Federal Rural University of Pernambuco, Recife, Brazil; Kumaun University, Nainital; Mayo Clinic Florida, USA; Miranda House - University of Delhi and Jawaharlal Nehru University, New Delhi

Our Objective

The primary objective of this conference is to bring together eminent experts from around the world at a single platform to drive advancements in the discovery and development of new therapeutics and radiopharmaceuticals for treating infectious diseases, neurological disorders, and cancer. We aim to provide a platform where interdisciplinary researchers can engage with esteemed speakers from institutions such as MIT-SMART, IITs, IISc, DBT labs, DRDO labs, University of California, BIOCEV Charles University, FIOCRUZ Brazil, Mayo Clinic Florida, RML Hospital, AIIMS, PGI Rohtak, and PGI Chandigarh. The conference seeks to foster cross- disciplinary collaboration between scientists, industry professionals, and physicians to enhance public health. This multidisciplinary event is designed to expose students and faculty members to global research challenges and to promote awareness among young research scholars and scientists from both research and clinical backgrounds. The conference will feature plenary and keynote lectures from renowned scientists and physicians, focusing on translational medicine, chemical sciences, and chemical biology, including panel discussions, workshops, flash talks, and poster presentations.

Scope

The conference will promote a cross-disciplinary collaboration between scientists, industry, and physicians toward a common goal of achieving better health for society. This multi-disciplinary conference is intended to expose students and young faculty members to the latest research methodologies, emphasizing addressing global problems. The scope of the conference is to sensitize, stimulate and create awareness among young research scholars and scientists from both translational research and clinical arena



SUCCESS STORIES

The previous two conferences, ICBTM-2019 and ICBTM-2022, were co-organized by Hansraj College - University of Delhi; Loyola University Chicago, USA; SGBT University Gurugram; Mayo Clinic Florida; Miranda House-University of Delhi; University of Debrecen, Hungary; Charles University Prague; and INMAS-DRDO have been resounding successes. These events were made possible through the generous sponsorship of DRDO, SERB, and DST.

ICBTM 2019






ICBTM 2022



MESSAGES

Dr. G. Satheesh Reddy,
President, AeSI
Former Secretary DD R&D,
Chairman-DRDO & Scientific
Adviser to Raksha Mantri

THE AERONAUTICAL SOCIETY OF INDIA

13-B, INDRAPRASTHA ESTATE, NEW DELHI-110002

Message

I am pleased to know that Hansraj College, University of Delhi is organizing 3rd International Conference on Integrative Chemistry, Biology and Translational Medicine (ICBTM-2024) from 08th to 10th March, 2024 in Udaipur, Rajsthan. I would like to convey my congratulations to Hansraj College, University of Delhi and other co-organizers, Pacific University Udaipur, a start-up company HeteroChem InnoTech on this occasion.

As the theme of the conference suggests, it will provide a dynamic platform for Chemists, Biologists and Pharma experts to deliberate upon how to translate the critical knowledge generated from basic R&D into more efficient drug development exercise. India has well established pharma industry of international standards; wealth of experienced basic science, pharma and clinical researchers; efficient research infrastructure and a diverse patient population making it an ideal place for innovative drug development. Research based consolidation and strengthening of Indian traditional medicine is also an important area to venture, and can provide a new fillip to Holistic Translational Medicine. These steps will strengthen "Atmanirbhar Bharat" and "Make for the World" initiatives. I strongly feel that a strong amalgamation of R&D programs amongst Institutions, Industry and Academia would ensure realization of India's true scientific potential in the field of drug discovery. The recent pandemic has proven that India has enormous untapped potential and can become a global leader in the area of drug development research.

I am confident that this conference will also serve as a launch pad for many young minds for sharing new ideas, brainstorm and collaborate for excellence in Translational Medicine. I wish the conference all the success, and extend my best wishes and greetings to the organizers and participants whose efforts have immensely contributed in shaping the conference.

Dr. G. Satheesh Reddy

Email: pres.aesi@gmail.com | Telefax: 011-23370768 | Web: www.aerosocietyindia.co.in

डॉ सुधीर चाँदना
निदेशक

Dr Sudhir Chandna
Director

सत्यमेव जयते

अ.स.प.सं. INM/DS/SC/02/2024
DO No.
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GOVERNMENT OF INDIA, MINISTRY OF DEFENCE
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BRIG. S. K. MAZUMDAR MARG, DELHI -110 054

27th Feb 2024

Message

I am delighted to know that Hansraj College, University of Delhi is organizing 3rd International Conference on Integrative Chemistry, Biology and Translational Medicine at Pacific University, Udaipur from 8th to 10th March 2024. I would like to convey my congratulations to organizers and co-organizers for organizing this conference for researchers working in these interdisciplinary areas.

India is referred as "Pharmacy of the world" due to mammoth export of affordable generic drugs, vaccines, and biologics across the globe. However, in this new era, we need to shift our gears and look forward to excel in the area of new drug discovery. The nationwide experience of managing COVID-19 in India has given immense experience and proven that we as a nation have enormous potential to become a global leader in the area of drug development research. Therefore, this is high time that our Biologists, Chemists and Pharma experts invest more resources and time in developing innovative new drugs and we move ahead from the generics. The success of country's drug discovery is closely linked to the collaboration between institutions, academia and industry. The conference is appropriately providing the platform for Chemists, Biologists and Pharma researchers from academia, institutions and industry to discuss and deliberate upon how to translate the innovative research in the form of new drugs and health care products.

I am confident that this Conference will provide a platform for knowledge exchange for researchers and many young minds to brainstorm and collaborate for excellence in Translational Medicine. I wish the conference a great success, and extend my best wishes and greetings to the organizers and participants whose efforts have contributed in organizing the conference.

(Dr. Sudhir Chandna)
Director

दूरभाष/Phone: +91 11-23905105 (O), फैक्स/Fax: +91 11-23919509, ई-मेल/E-mail: director.inmas@gov.in

Reg. No. : 45/UDR/95-96

PACIFIC ACADEMY OF HIGHER EDUCATION & RESEARCH SOCIETY

PIT Campus, " Pacific Hills " Airport Road, Pratap Nagar, Udaipur (Raj.)

Ph. : +91-294-2494520, Fax : +91-294-2494519, Website : www.pahersociety.org

Greetings and Best Wishes for ICBTM-2024

Dear Esteemed Participants,

It is my pleasure to extend a heartfelt welcome to all attendees of the International Conference on Integrative Chemistry, Biology, and Translational Medicine 2024 (ICBTM-2024) on behalf of the PAHER Society, Udaipur. As the Chairperson, I am excited about the collaborative efforts between Hansraj College, Delhi University, and Pacific University, Udaipur, in organizing this noteworthy event.

The exemplary partnership with prestigious entities such as HetroChem InnoTech, Oswaldo Cruz Foundation, Charles University, University of Debrecen, and Mayo Clinic, among others, underscores our collective commitment to advancing interdisciplinary research on a global scale.

The distinguished keynote speakers and representatives from esteemed institutions, including Loyola University, Jawaharlal Nehru University, and the University of Ghana, promise to bring a wealth of knowledge and insight to the conference. Their contributions will undoubtedly shape discussions and inspire innovative approaches in chemistry, biology, and translational medicine.

Udaipur, with its rich cultural tapestry, serves as a fitting backdrop for fostering meaningful connections and intellectual exchanges. I am confident that ICBTM-2024 will serve as a catalyst for ground breaking ideas and collaborative initiatives that will redefine the landscape of these disciplines.

To all participants, I extend my best wishes for a successful and enriching conference. May your interactions and engagements during this event lead to profound discoveries, foster innovation, and establish enduring partnerships.

Thank you for being a part of this momentous occasion, and I eagerly anticipate the transformative discussions and outcomes that will emerge from ICBTM-2024.

Warm regards,

Bholaram Agarwal

Chairman

PAHER Society, Udaipur, India

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NAAC ACCREDITED 'A++' GRADE COLLEGE

Message

Hansraj College, University of Delhi, a premier institution of higher education in India, takes pride in organizing the 3rd International Conference on "Integrative Chemistry, Biology and Translational Medicine (ICBTM-2024) in a potential cooperation of Pacific University Udaipur, and HeteroChem InnoTech (an ingenious startup), which is scheduled from 8th to 10th March. I am glad that Hansraj College has maintained the continuity of organizing ICBTM since 2019.

Hansraj College, University of Delhi has always been responsible for providing its students with quality education by providing them with highly qualified and academically enriched faculty, first-rate infrastructure and stellar technology for all students. It has always kept the requirements of its students as its frontier priority and worked towards constantly improving student progression. The college has always kept pace with the development in all sectors of education, including the introduction of any newly developed methods of teaching, such as the implementation of the recently introduced multidisciplinary teaching coverage, NEP (New Education Policy) 2020, intending to enhance any skills fostering in the students of Hansraj. Considering this approach to the all-rounded development of a student, it has also actively organised induction programmes, conferences, seminars, symposia etc.

Hence, it fills my heart with immense pride to bring forward this golden opportunity for all budding scientists and academic enthusiasts in Hansraj College to organize the ICBTM 2024 Conference 3.0. I am confident that this Conference will provide a platform for knowledge exchange and discussion of the latest research methodologies and recent developments in the above-mentioned fields, thereby giving students and faculties an elbow room to enrich themselves in their areas of interest.

Congratulating and wishing the best to all members of the organizing team, as well as every student actively attending, for the great success of this conference.

Prof. (Dr.) Rama
Principal &
Chairman ICBTM 3.0

PACIFIC ACADEMY OF HIGHER EDUCATION AND RESEARCH UNIVERSITY, UDAIPUR

Warm Welcome and Best Wishes for ICBTM-2024

Dear Esteemed Participants,

It is with great pleasure and enthusiasm that I extend my warmest welcome to each one of you on behalf of Pacific University, Udaipur. As the Chairperson, I am delighted to witness the collaboration and confluence of minds at the International Conference on Integrative Chemistry, Biology, and Translational Medicine 2024 (ICBTM-2024).

This conference, organized in exemplary partnership with Hansraj College, Delhi University, and co-hosted by Pacific University, Udaipur, reflects a shared commitment to advancing knowledge and fostering global collaboration in the fields of chemistry, biology, and translational medicine. The association with esteemed partners like HetroChem InnoTech, Oswaldo Cruz Foundation, Charles University, University of Debrecen, Durban University of Technology, and Mayo Clinic among others, demonstrates the diverse and international nature of this event.

We are honoured to have representatives from renowned institutions and distinguished keynote speakers from around the world contributing their expertise. The knowledge, insights, and experiences that will be shared during this conference promise to be transformative, inspiring innovative thinking and ground breaking research.

As we gather in Udaipur, a city known for its rich cultural heritage, I am confident that the exchange of ideas, collaborations, and discussions during ICBTM-2024 will contribute significantly to the advancement of integrative approaches in chemistry, biology, and translational medicine.

I extend my best wishes to all participants for a successful and intellectually enriching conference. May this gathering be a source of inspiration, fostering meaningful connections and opening new avenues of exploration and discovery.

Thank you for being a part of this collaborative endeavor, and I look forward to the exciting discussions and outcomes that will emerge from ICBTM-2024.

Warm regards,

Rahul Agarwal

Chairperson

Pacific University, Udaipur, India

Pacific Hills, Pratapnagar Extension, Airport Road, Debari, Udaipur - 313024 (Rajasthan)
Phone : 0294-2665000 | info@pacific-unicersity.ac.in

HG Khorana Centre For Chemical Biology
Department of Chemistry, Hansraj College
University of Delhi, Delhi -110007 India.
Tel: +91-11-27667458, Email: brijeshrathi@hrc.du.ac.in

Message

Founder & CEO, HeteroChem InnoTech &
Associate Professor of Chemistry

I am delighted to be able to bring forward the 3rd International Conference on Integrative Chemistry, Biology and Translational Medicine (ICBTM 3.0) as a joint event of Hansraj College, University of Delhi; HeteroChem InnoTech & Pacific University Udaipur in exemplary collaboration of partnership with University of Debrecen, Hungary; Mayo Clinic Florida, USA; Oswaldo Cruz Foundation (Fiocruz) Recife, Brazil; Charles University, Czech Republic; Federal Rural University of Pernambuco, Brazil; Kumaun University Nainital; Miranda House, University of Delhi & Jawaharlal Nehru University, New Delhi. The conference is scheduled from 8th to 10th March 2024 at Pacific University Udaipur, Rajasthan.

Hansraj College and HeteroChem InnoTech (startup, a new era in drug discovery) have worked together before to bring forward ICBTM-2022, and it has been a huge success both times. We hope to uphold this platform for exchanging ideas regarding translational medicine and integrative biology with scientists worldwide. This conference will provide the attendees with newly developed knowledge and facts in modern medicine and inspire students to join the research sector as it is the most important sector of the scientific community. The youth of Bharat must be educated regarding all the advancements in these fields.

I hope the students and participants benefit from all the speaker sessions and panel discussions. I also convey my best wishes to the organizing committee and wish for the conference's success!

Dr. Brijesh Rathi
Convener, ICBTM 3.0

SCIENTIFIC PROGRAMMME

3rd International Conference of Integrative Chemistry, Biology & Translational Medicine

ICBTM 3.0

March 8-10, 2024
Udaipur, Rajasthan
Bharat

Organizers

Hansraj College, University of Delhi, Delhi, Bharat
Pacific University Udaipur, Rajasthan, Bharat
HeteroChem InnoTech Private Limited, Bharat

venue: Pacific University, Debari, Udaipur

web: icbtmconference.com

PRE CONFERENCE WORKSHOP

ICBTM 3.0 venue: Pacific University, Udaipur

March 7, 2024

15:00 – 16:30

Navigating opportunities
A Guide to Effective Communication Skills

Pawan K. Dhar, Ph D
Professor & Head
Synthetic Biology Group
School of Biotechnology
Jawaharlal Nehru University, New Delhi

16:30 – 18:00

Artificial Intelligence in Biology

Binay Panda, Ph D
Professor & Head
Computational Genomics Group
School of Biotechnology
Jawaharlal Nehru University, New Delhi

workshop venue: Computer Lab, Pacific College of Engineering

CONFERENCE SCHEDULE

ICBTM 3.0 Pacific University

Day 1: March 8

07:00 – 08:20 Registration | Tea | Coffee

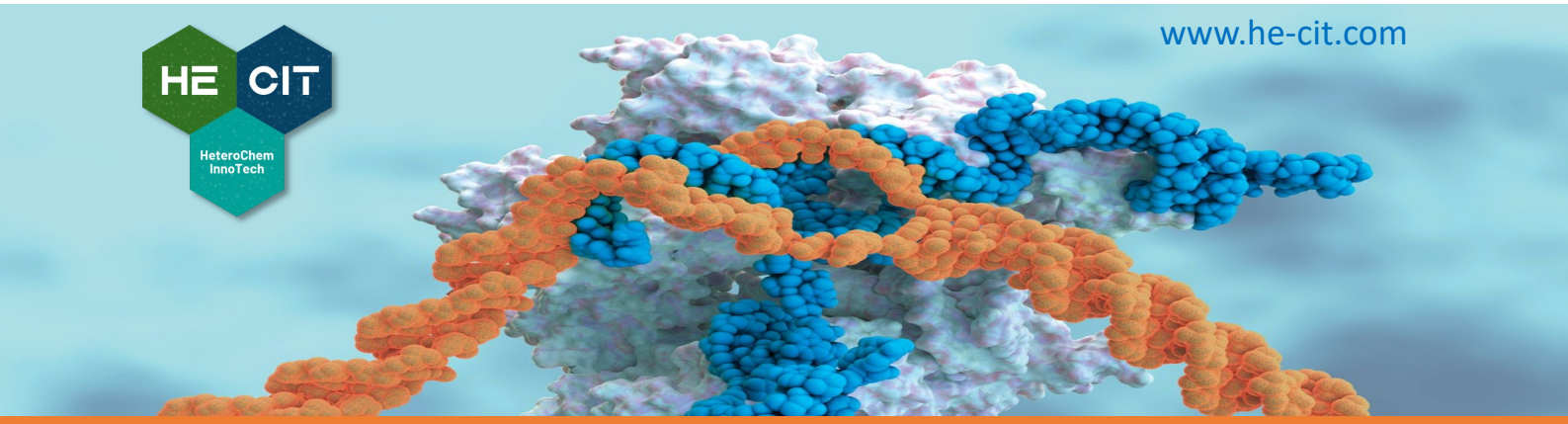
08:30 – 09:35 Inaugural Ceremony

09:40 – 10:20 Inaugural Lecture

Chair
Dr. Sudhir Chandna, Director & Sc 'G', Institute of Nuclear Medicine and Allied Sciences (INMAS), Defence Research and Development Organisation (DRDO), Government of Bharat

Prof. Julien Lescar

Professor & Director, NTU Institute of Structural Biology, Singapore &
Principal Investigator, Singapore-MIT Alliance for Research and Technology Centre, Singapore
Title: Using the Cellular Thermal Shift Assay Combined with Structural Biology to Identify and Validate Malaria Drug Targets.



HeteroChem InnoTech
a new era in drug discovery

CONFERENCE SCHEDULE

ICBTM 3.0

Venue: Pacific University

Day 1: March 8

HALL - A

Theme: Biology of Infectious Diseases & Drug Discovery

Chair & Co-chair

Prof. Pawan K Dhar, Jawaharlal Nehru University, Delhi.
Prof. KK Dave, President, PAHER, Udaipur.

Prof. Anil Chuturgoon 10:35 – 11:10
University of KwaZulu-Natal, South Africa
Title: Patulin induced nephrotoxicity - a mechanistic overview

Prof. Satish K Awasthi 11:15 – 11:50
Department of Chemistry, University of Delhi, Bharat
Title: Recent advances in Antimalarial drug discovery : Past, Present and Future

Prof. Pawan K. Dhar 11:55 – 12:25
Jawaharlal Nehru University, New Delhi, Bharat
Title: Dark Genome - a new drug discovery platform

Dr. Vera Alferova 12:30 – 13:00
Russian Academy of Sciences, Russia
Title: Current Trends in Natural Antibiotic Discovery

HALL - B

Theme: Chemistry of Bioactive Molecules

Chair & Co-chair

Prof. Suresh C Ameta, Professor Emeritus, Pacific University, Udaipur
Prof. Hemant Kothari, Dean, PG Studies, Pacific University, Udaipur

Prof. Akhilesh K Verma 10:35 – 11:10
Department of Chemistry, University of Delhi, Bharat
Title: Real-Time Monitoring Organic Reactions: Mechanistic Analysis of Reaction Intermediates/Species Using Online Mass Spectrometer

Prof. K. Rajshekhar 11:15 – 11:50
University of KwaZulu-Natal, South Africa
Title: Palladium-Catalyzed Regio divergent C-H Olefination of Imidazo[1,2a] pyridine Carboxamide and Unactivated Alkenes

Dr. Bakai-Bereczki Ilona 11:55 – 12:25
University of Debrecen, Hungary
Title: Glycopeptide antibiotic derivatives against viruses

Prof. Ashutosh K. Mishra 12:30 – 13:00
Indian Institute of Technology, Hyderabad
Title: Modulating intrinsic behavior of the flavin core for biological applications

HALL - C

Theme: Global Health & Challenges

Chair

Prof. Ravi Durvasula, Chair of Infectious Diseases, Mayo Clinic, Florida, USA

Prof. Ravi Durvasula & Dr. Prakasha Kempaiah 10:35 – 11:15
Mayo Clinic Florida, USA.
Title: Immunobiology of Long COVID-19 Syndrome

Dr. Pulin K. Gupta 11:15 – 11:45
Dr. Ram Manohar Lohia Hospital (RML), Delhi, Bharat
Title: Management of dengue fever and malaria--current scenario and counteracting strategies in India

Dr. Rohit Chitale 11:45 – 12:15
Mayo Clinic Florida, United States of America.
Title: Artificial Intelligence Will Change Humanity Forever: Proactive Health Solutions For Disease Prevention

Dr. Atulabh Vajpayee 12:25 – 13:00
Neurologist, Pacific Medical College and Hospital, Pacific Medical University, Udaipur Bharat
Title: Advances in Neurochemistry

13:00 – 14:00 LUNCH & POSTER SESSION

Chair

Prof. Dilendra Hiran, Chairman, S&T, Pacific University, Udaipur, Bharat

Prof. Mandira Varma Basil 14:00 – 14:30
Patel Chest Institute, DU, Bharat
Title: Unveiling the importance of Nontuberculous Mycobacteria as potential human pathogens

Dr. Vinoth Rajendran 14:30 – 15:00
Pondicherry University, Bharat
Title: Zinc Pyrithione Inhibits Blood Stage Parasites of Plasmodium falciparum in Culture

Chair

Prof. P.K. Chaudhary, Dean, Faculty of Pharmacy, Pacific University, Udaipur, Bharat

Prof. Ram Sagar 14:00 – 14:25
JNU, New Delhi, Bharat
Title: Metal-free Synthesis of Natural Product-Inspired Glycohydrids as Anticancer Agents

Dr. Neeraj Mishra 14:25 – 14:45
Lucknow University, Bharat
Title: Catalyst-Controlled C–H Allylation and Annulation of (Hetero)arenes Using Cyclic Carbonates

Dr. Parvin Jangra 14:45 – 15:00
Kurukshetra University, Haryana, Bharat
Title: CORAL - Identification of structural attributes of cannabinoid receptor-1 antagonists compounds using correlation contradiction index

Chair

Prof. Mahendra Rana, Kumaun University Nainital, Uttrakhand, Bharat

Dr. Sinka David 14:00 – 14:30
University of Debrecen, Hungary
Title: The Importance of Collaboration Between Academia and Industry in Pharmaceutical R&D

Dr. Prerna Sharma 14:30 – 15:00
Institute of Human Behaviour & Allied Sciences (IHBAS), Delhi, Bharat
Title: Youth Mental Health - Imagining Safer and Enabling Spaces for Young People

SIGHTSEEING

15:00 – 19:00

City Palace

Jagdish Temple

Shilpgram

ICBTM 3.0

CONFERENCE SCHEDULE

venue: Pacific University

Day 2: March 9

09:00 – 09:40

HALL - A

Plenary Lecture

Chair: **Prof. Aniko Borbas**, University of Debrecen, Debrecen, Hungary

Prof. Peter Preiser

MIT-SMART & NTU, Singapore

Title: Role of the Epitranscriptome in Posttranscriptional Regulation of Expression in Malaria Parasites

09.45 – 9.55 TEA | COFFEE

HALL - A

Theme: Biology of Infectious Diseases & Drug Discovery

Chair

Prof. DS Rawat, Vice Chancellor, Kumaun Univ., Bharat

Dr. Lindomar Pena 10:00 – 10:35
Principal Investigator, AggeuMagalhaes Institute (IAM), Recife, Brazil
Title: Antiviral Discovery Against Emerging Viruses

Prof. Rupesh Chaturvedi 10:40 – 11:15
Jawaharlal Nehru University, New Delhi, Bharat
Title: Single Cell-Drived Spheroids: A Tool to Capture Functional and Genetic Heterogeneity

Dr. Satish Mishra 11:20 – 11:50
CSIR Central Drug Research Institute, Lucknow, Bharat
Title: The multifunctional autophagy pathway as a potential drug target for malaria

Dr Ferenc D. Petroczi 11:55 – 12:30
University of Debrecen, Hungary
Title: Synthesis of fluorine-containing Cannabinoid Derivatives with various biological activities

HALL - B

Theme: Chemistry of Bioactive Molecules

Chair

Prof. S.K. Verma, Pacific Medical College and Hospital, Pacific Medical University, Udaipur

Prof. Ronaldo Oliveira 10:00 – 10:35
UFRPE, Recife, Brazil
Title: Carbohydrate-based Small Molecules Derivatives: Stay on the Roads Toward Bioactive Compounds

Prof. B.K. Singh 10:40 – 11:15
Department of Chemistry, Univ. of Delhi, Bharat
Title: Regioselective Chalcogenation of Quinoxolinones and Benzoxazines *via* C-H activation

Prof. I. K. Singh 11:20 – 11:50
DBC, University of Delhi, Bharat
Title: ZINC1250228067: A Promising Therapeutic for Permanent Vision Loss.

Prof. Ramendra Pratap 11:55 – 12:30
Department of Chemistry, Univ. of Delhi, Bharat
Title: Synthesis of various functionalized Aza heterocycles from aryl methyl ketones of biological importance

HALL - C

Mini Invited Talks

Chair

Prof. M.M. Mangal, Principal, Pacific Medical College & Hospital, Pacific Medical University, Udaipur

Dr. Richard Kajtar 10:30 – 10:50
University of Debrecen, Hungary
Title: Pharmacological Research of Newly Synthesized CBD Derivatives.

Dr. Vijay K Goel 10:50 – 11:05
Jawaharlal Nehru University, New Delhi, Bharat
Title: Leveraging Bioinformatics Tools for the Discovery of Novel Anti-Malarials.

Dr. Kapil Vashisht 11:05 – 11:20
HeteroChem InnoTech, Delhi Bharat
Title: Rapid Diagnostic Tests (RDTs) for malaria: why we need new targets now?

Dr. Soumyananda Chakraborty 11:20 – 11:35
ICMR-National Institute of Malaria Research, Bharat, Bharat
Title: Antimalarial delivery with ferritin-based protein cage: A step towards developing smart therapeutics against malaria

Dr. Pawan Kumar 11:35 – 11:45
Rajdhani College, University of Delhi, Bharat
Title: Secondary Phosphine Chalcogenides Decorated Gold Nanoparticles as Potential Antiparasitic Agents.

Dr. Bhupesh Goyal 11:45 – 11:55
Thapar Institute of Engineering and Technology, Bharat
Title: Illuminating the destabilization mechanism of small-molecule inhibitors against α–Syn oligomers in Parkinson's disease using molecular dynamics simulations

Dr. Manisha Vajpayee 11:55 – 12:05
Pacific IVF centre, Pacific Medical College and Hospital, Pacific Medical University, Udaipur Bharat
Title: Gut microbiota influencing fertility

Dr. Deepender Kaushik 12:05 – 12:20
University of Nebraska Medical Center, USA
Title: TBA

Dr. Sunil Kumar 12:20 – 12:30
University of Nebraska Medical Center, USA
Title: Synthesis of 2-Aminothiazole Functionalized Imidazo[1,2-a]pyridines via Transition-Metal Free Approach as Novel Antibacterial Agents

12:30 – 13:30 LUNCH & POSTER SESSION

Pacific University
Udaipur, Rajasthan

Pacific Medical University
Udaipur, Rajasthan

ICBTM 3.0

CONFERENCE SCHEDULE

venue: Pacific University

Day 2: March 9

HALL - A

Theme: Biology of Infectious Diseases & Drug Discovery

Chair

Prof. Anil Chuturgoon, University of KwaZulu-Natal, South Africa

Dr. KC Pandey 13:30 – 14:00
ICMR-National Institute of Malaria Research, Bharat
Title: Recent update on antimalarials; Parasite proteases are potential target.

Dr. Agam P Singh 14:00 – 14:30
National Institute of Immunology, New Delhi, Bharat
Title: HEA (hydroxyethylamine) based potent and safe anti-malarials.

Dr. Anant N. Bhatt 14:30 – 15:00
Scientist 'F', INMAS-DRDO, Delhi, Bharat
Title: Upregulation of energy metabolism and pro-inflammatory signaling confers radio-protection in in-vitro and in-vivo small animal models.

Prof. Ajeet Jaiswal 15:05 – 15:30
DHSGSU, Bharat
Title: Indigenous Knowledge of Healing Among the Tribes.

HALL - B

Theme: Chemistry of Bioactive Molecules

Chair

Prof. K. Rajshekhar, University of KwaZulu-Natal, South Africa

Dr. Siew Pheng Lim 13:30 – 14:00
Singzyme Pte. Ltd., Singapore
Title: PALs: high-speed precision bio-conjugation

Dr. Alexey Ustinov 14:00 – 14:30
Russian Academy of Sciences, Russia
Title: Current Trends in Photosensitizing Antiviral Drugs

Prof. Sadhna Sharma 14:30 – 15:00
MH, University of Delhi, Bharat
Title: Diagnostic and Vaccine potential of early and late protein antigens of Mycobacterium tuberculosis.

Dr. Alexandra Gyongyosi 15:00 – 15:30
University of Debrecen, Hungary
Title: BGP-15 protects against doxorubicin-induced cell toxicity via enhanced mitochondrial function (Invited).

HALL - C

Mini Invited Talks

Chair

Dr. Anant N Bhatt, Sc 'F' INMAS-DRDO, Delhi, Bharat

Dr. Priyamvada Singh 13:30 – 13:45
MH, University of Delhi, Bharat
Title: SARS-CoV-2: Efforts for the drug design & drug discovery.

Dr. Monika Sharma 13:45 – 14:00
MH, University of Delhi, Bharat
Title: PE/PPE family proteins of Mycobacterium tuberculosis modulate host cellular pathways as molecular mimics of host proteins.

Dr. Shikha Agarwal 14:00 – 14:15
MLSU, Udaipur, Bharat
Title: Exploring the Unique Usage of g-C3N4.SO3H Ionic Liquid as an Efficient Catalyst for One-Pot Synthesis of Biologically Active 1,1-Dihomoarylmethane Scaffolds.

Dr. Mansi Verma 14:15 – 14:30
Hansraj College, University of Delhi, Bharat
Title: Exploring Dengue Virus: multi-omics approach using in silico studies.

Dr. Sohan Lal 14:30 – 14:45
Kurukshetra University, Haryana, Bharat
Title: Preparation of Food Packaging Films Based on O-Carboxymethyl Chitosan/PVA/Hemp fiber Filled with Neem extract: Mechanical, Antimicrobial and Biodegradation Studies

15:05 – 16:00 PANEL DISCUSSION

HALL - A

"Next Wave of Drug Discovery: Opportunities & Challenges"

Moderator: **Prof. Rupesh Chaturvedi**, Jawaharlal Nehru University, New Delhi, Bharat
Panelists: Prof. Peter Preiser, MIT-SMART & NTU, Singapore
Dr. Siew Pheng Lim, Experimental Drug Development Centre (EDDC), A*STAR, Singapore
Prof. Ravi Durvasula, Chair of Infectious Diseases, Mayo Clinic, Florida, USA

16.00 – 16.30 TEA | COFFEE

16:30 – 17:10 Keynote Lecture

Chair: **Prof. Rohit Chitale**, Mayo Clinic Florida, USA

HALL - A

Prof. DS Rawat

Senior Professor of Chemistry, DU; Vice Chancellor, Kumaun University Nainital, Uttrakhand, Bharat
Title: Navigating the Expected and Unexpected Twists and Turns of Lead Optimization: The Discovery of Clinical Candidate for the Treatment of Parkinson's Disease.

17:10 – 18:00 Tips and Tricks for Academic Networking

venue: Pacific University

18.00 – 19.00 **Rajasthani Cultural Event**

19.00 – 20.30 **Dinner**

ICBTM 3.0

CONFERENCE SCHEDULE

venue: Pacific University

Day 3: March 10

HALL - A

09:00 – 09:40

Plenary Lecture

Chair: **Prof. Lescar Julien**, MIT-SMART, NTU Singapore

Prof. Aniko Borbas

Head, Department of Pharmaceutical Chemistry, University of Debrecen, Hungary.

Title: Sugar-Modified Nucleoside Analogs with Anticancer, Antiviral and Antimalarial Activity

09.45 – 10.00 TEA | COFFEE

10.00 – 12.00

ORAL PRESENTATIONS

HALL - A	HALL - B	HALL - C	HALL - D
OP 1- 10	OP 11- 30	OP 31- 50	OP 31- 50

HALL - A 12:00 – 13:30

Workshop

on

"ROLE OF STRESS MANAGEMENT IN PSYCHOSOMATIC (SOMATOFORM) DISORDER"

Mentor: Dr. Deepak K Salvi & team, Professor & Head, Pacific Medical College & Hospital, Udaipur

13:30 – 14:30 LUNCH

14:35 – 15:30

Certificate Distribution, Awards, Valedictory, Vote of Thanks

Hansraj College
University of Delhi

SPEAKERS' ABSTRACTS

Beyond the Bench: Mastering the Art of Communication

Prof. Pawan K. Dhar

Head, Synthetic Biology Group School of Biotechnology,
Jawaharlal Nehru University,
New Delhi, Bharat

Abstract

Whether you're presenting groundbreaking research to colleagues or explaining complex ideas to the public, effective communication is the hallmark of a successful scientist. Join us for this engaging tutorial where you'll learn to transform your scientific jargon into captivating stories that resonate with any audience. Master the art of storytelling to weave your research findings into clear narratives that engage your audience. Gain practical tips and strategies to overcome nervousness and deliver confident and engaging presentations. This interactive workshop is open to researchers at all stages of their careers. Through a combination of interactive exercises you will learn how to write an effective cover letter, perform in interviews and group discussions, build a professional CV and deliver an impactful talk.

 ISBN: 978-93-95033-37-4

Artificial Intelligence in Biology

Prof. Binay Panda

Head Computational Genomics Group, School of Biotechnology,
Jawaharlal Nehru University, New Delhi, Bharat

Abstract

Biology is undergoing a transformative revolution fueled by Artificial Intelligence (AI). This tutorial will explore frontiers of this dynamic field and discovering how AI is empowering biologists to delve into the world of genomics, proteomics, and beyond, where AI deciphers massive datasets, uncovering hidden patterns and accelerating research. Explore how AI aids in drug discovery, and personalized medicine, paving the way for more effective treatments. This interactive tutorial is designed for participants of all levels, from students eager to embrace new a to seasoned researchers seeking to expand their horizons. Through clear explanations, engaging examples, and hands-on exercises, you will gain a solid understanding of core AI concepts and techniques relevant to biology.

 ISBN: 978-93-95033-37-4

Using the Cellular Thermal Shift Assay combined with Structural Biology to Identify and Validate Malaria Drug Targets

Julien Lescar [a,b,c], Jianqing Lin [a,b], Zara Chung [a,b], Grennady Wirjanata[a] , Jerzy M Dzekian [a], Peter Preiser[a] and Zbynek Bozdech[a,b]

[a] School of Biological Sciences, Nanyang Technological University, 60 Nanyang Drive, 637551 Singapore [b] NTU Institute of Structural Biology, Nanyang Technological University, Experimental Medicine Building (EMB), 59 Nanyang Drive, Level 06-01, 636921 Singapore
[c]Antimicrobial Resistance Interdisciplinary Research Group, Singapore-MIT Alliance for Research and Technology Centre, 1 CREATE Way, 138602 Singapore
Present address: Walter and Eliza Hall Institute of Medical Research, Melbourne, Victoria, Australia
julien@ntu.edu.sg

Abstract

Plasmodium falciparum accounts for the majority of the estimated 400,000 deaths caused by malaria every year. In the absence of an efficacious vaccine, chemotherapy remains key to prevent, treat and contain this disease. A worrying trend is that the continuous decrease in deaths observed in the last twenty years is now slowing down, with the number of malaria cases reaching a plateau over the 2021-2023 period [1]. In addition, the efficacy of several drugs currently used in the clinic is suffering from the emergence of resistant parasites. Therefore, global efforts to identify novel lead compounds to treat malaria are underway, such as the Glaxo-SmithKline Tres Cantos antimalaria set and the Medicine for Malaria Ventures (MMV), which are repositories of molecules able to kill the parasite in cell-based assays. While phenotypic screens provide indispensable libraries of leads to combat malaria, often, little is known about the mechanism of action employed by these compounds to kill the parasite. Likewise, the precise mechanism of actions of many drugs used in the clinic remains poorly defined.

We used mass spectrometry coupled with the cellular thermal shift assay (MS-CETSA) to identify putative protein targets from MMV compounds such as MMV000848 [2], of orally active investigational new drugs such as MK-4815 from Merck [3] and also of drugs used in the clinic [4]. In each case, binding and inhibition assays were complemented by 3D structure determination of the putative proteins targets, bound with the compound, using either X-ray crystallography [2,4] or cryo-EM. Moreover, when possible, drug sensitivity was also tested on knock-down or knock-out strains compared to the wild-type 3D7 strain. Taken together, these results identified several targets including purine nucleoside phosphorylase or falcilysin in the hemoglobin digestion pathway and suggest avenues to improve inhibitor potency.

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Role of the Epitranscriptome in Posttranscriptional Regulation of Expression in Malaria Parasites

Peter Preiser [a, b]

[a] School of Biological Sciences, Nanyang Technological University, Singapore,
[b]Antimicrobial Resistance Interdisciplinary Research Group, Singapore-MIT Alliance for Research and Technology, Singapore
*prpreiser@ntu.edu.sg

Abstract

The post-transcriptional regulation of translation by the dozens of modified nucleosides in RNA – the epitranscriptome – has recently been recognized as a key additional step that impacts on cell function and biology. The epitranscriptome can play a role both at the level of mRNA modifications as well as tRNA modifications. Recent work has shown that the dynamic regulation of tRNA modifications coupled with codon-biased gene families has a direct impact on the translational capacity of a cell. Changes in tRNA modifications have been shown in particular to be important factors in cellular stress responses.

The malaria parasite Plasmodium falciparum remains one of the most important infectious diseases globally, causing huge tolls both in terms of morbidity and mortality. The genome of the parasite has revealed several striking features including the lack of an extensive transcriptional regulatory capacity as well as a relatively small number of tRNA genes. While all nuclear-encoded tRNAs in P. falciparum are like other eukaryotic tRNAs in terms of semi-conserved sequences and structure, the parasite has the smallest set of tRNA genes for a eukaryotic cell, with only one gene copy per tRNA isoacceptor for the nuclear genome. This unique characteristic of P. falciparum highlights the potential importance of epitranscriptomic modifications in a complex regulatory network that accurately decodes 61 codons by 45 cytoplasmic tRNA iso-acceptors. Our studies on the human malarial protozoan pathogen, Plasmodium falciparum have shown that both mRNA and tRNA modifications drive translation of specific transcripts to ensure progression of the parasitic developmental cycle. Importantly, we now provide evidence that tRNA modification changes play an important role in parasite stress response and potentially represent another layer of complexity in the parasites ability to overcome specific drug pressure. In addition, it is apparent that enzymes involved in regulating these modifications represent attractive new targets for drug development. My talk will focus on the current understanding of tRNA modifications in P. falciparum and their role specifically in stress response and drug resistance.

 ISBN: 978-93-95033-37-4

Sugar Modified Nucleoside Analogs with Anticancer, Antiviral and Antimalarial Activity

Anikó Borbás [a,b,c]

[a]Department of Pharmaceutical Chemistry, University of Debrecen, Egyetem tér 1, H-4032 Debrecen Hungary,
[b]2HUN-REN-UD Molecular Recognition and Interaction Research Group, University of Debrecen, Hungary
[c]National Laboratory of Virology, University of Pécs, Hungary
borbas.aniko@pharm.unideb.hu

Abstract

Nucleoside analogs, which are chemically modified derivatives of natural nucleosides, have been key medicines in the treatment of cancer and viral diseases for decades, and are also used in antiprotozoal, antifungal, and antibacterial therapy.[1] For therapeutic applications, nucleosides are typically modified at the ribose sugar or the nucleobase. Important representatives of nucleoside analogs are morpholinos (morpoline-ring nucleosides), which contain a morpholine heterocycle instead of the native ribofuranose ring.

Recently, we have developed efficient synthetic methods for the preparation of new types of sugar-modified nucleoside analogs, which can be divided into two large groups. The first group includes new morpholino-type nucleoside analogs, which instead of the ribofuranose unit contain an N-fluoroalkylated morpholine ring or different bi- and tricyclic ring systems. The synthetic strategy was based on oxidative ring cleavage of the vicinal diol unit in ribofuranose of nucleosides, followed by cyclization of dialdehyde intermediates with various functionalized amines, including fluorinated primary amines. [2,3] The second group of sugar-modified nucleosides includes configurationally altered, L-lyxo, D-xylo or D-arabino configured nucleoside derivatives bearing a sulfanylmethyl-linked substituent at different positions of the furanose ring. These derivatives were prepared by photoinitiated radical addition of various thiols onto C4', C3' or C2' exomethylene moiety of nucleosides. [4-6]

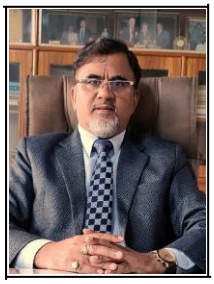
Among the above nucleoside derivatives, we have identified several anti-tumor, anti-SARS-CoV-2 and anti-malarial compounds. [5-7] In this lecture, the synthesis, biological evaluation and SAR study of the novel nucleoside analogs will be presented.

References:

[1] L. P. Jordheim, D. Durantel, F. Zoulim, C. Dumontet. Nat. Rev. Drug Discov. 2013, 12, 447–464.
[2] N. Debreczeni, M. Bege, M. Herczeg, I. Bereczki, G. Batta, P. Herczegh, A. Borbás. Org. Biomol. Chem. 2021, 19, 8711-8721.
[3] N. Debreczeni, J. Hotzi, M. Bege, M. Lovas, E. Mező, I. Bereczki, P. Herczegh, L. Kiss, A. Borbás. Chem. Eur. J. 2023, 29, e202203248

 ISBN: 978-93-95033-37-4

Navigating the Expected and Unexpected Twists and Turns of Lead Optimization: The Discovery of Clinical Candidate for the Treatment of Parkinson's Disease



Diwan S Rawat

Senior Professor of Chemistry, University of Delhi & Vice Chancellor, Kumaun University, Nainital-263601, Uttrakhand, Bharat

Abstract

In order to address the issue of drug resistance and improve the ADME properties of a drug molecule concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule. This approach may lead to a molecule with improved efficacy and may solve the problem of drug resistance and reduce the undesired side effects [1,2]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine phamacohpore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studies for Nurr1 activation, a potential target for Parkinson disease model and identified 15 hits out of which 3 compounds have cleared pre-clinical trials and technology has been transferred to NURRON pharmaceuticals for further development [3-10]. These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of α-synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cures the Parkinson induced mice model at 5 mg/kg body weight without any toxicity and recently phase I clinical trials of one of the molecules have begun.

References:

1. B. Meunier, B. Acc. Chem. Res. 2008, 41, 2008.
2. S. S. Shikha, M. Sharma, P.M.S. Chauhan, Drug News & Perspective, 2010, 23, 632.
3. S. Manohar, D. S. Rawat, ACS Med. Chem. Lett. 2012, 3, 555.
4. Beena, K. K. Raj, S. M. Siddiqui, A. Azam, D. S. Rawat, Chem. Med. Chem. 2014, 9, 2439.
5. A. Thakur, S. Manohar, V. Kumar, S. V. Malhotra, D. S. Rawat, Med. Chem. Commun. 2014, 5, 576.
6. M. Tripathi, D. Taylor, S. I. Khan, B. L. Tekwani, P. Ponnan, T. Velpandian, U. Das, D. S. Rawat, ACS Med. Chem. Lett. 2019, 10, 714.

Patulin Induced Nephrotoxicity- A Mechanistic Overview

Yashodani Pillay, Terisha Ghazi, Savania Nagiah, Makabongwe Mazibuko, and Anil Chuturgoon*

Discipline of Medical Biochemistry, College of Health Sciences, University of KwaZulu-Natal, South Africa
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Abstract

Patulin (PAT) is a food-borne mycotoxin produced by *Penicillium* and *Byssochlamys* species. It is widely known for its mutagenic, carcinogenic, and genotoxic effects and has been associated with kidney injury; however, the mechanism of toxicity remains unclear. PAT is a common contaminant of apples and apple products, and has recently been implicated in nephrotoxicity, impaired metabolic and kidney function [*1*].

Our studies focused on mechanisms of PAT toxicity using an in vitro kidney cell line (HEK293) and mice. We found that PAT induced oxidative stress, compromised mitochondrial function and caused cell death via depletion of the antioxidant GSH in HEK293 cells [*2*]. Further PAT activated the NRF2 antioxidant response that was enhanced by SIRT3 [*3*]. PAT influenced changes in lipid metabolism and inflammation, and altered the epigenetic environment [*4*]. PAT-induced decreases in transcription and translation of α_1-adregergenic receptor (AR) was associated with changes in downstream PI3K and MAPK signaling [*5*].

Further, we explored the changes in α-AR signalling pathways and epigenetic modifications induced by PAT in the kidneys of C57BL/6 mice during acute. PAT downregulated the expression of *ADRA1*, *ADRA2A*, *ADRA2B*, *PI3K*, and *AKT* and upregulated ERK1/2 and MAPK protein expression. PAT induced alterations in DNA methylation patterns by upregulating DNMT1 expression and downregulating DNMT3A, DNMT3B, and MBD2 expressions, resulting in global DNA hypomethylation [7].

In conclusion, PAT disrupts α -1 and α -2 AR signalling pathways and induced epigenetic modifications, leading to kidney injury.

References:

[1] Pillay Y, Phulukdaree A, Nagiah S, Chuturgoon AA. Toxicon, 2015, 99, 1-5
[2] Pillay Y, Nagiah S, Krishnan A, Chuturgoon AA. Sci Rep, 2020, 10(1), 20115
[3] Pillay Y, Ghazi T, Raghubeer S, Nagiah S, Chuturgoon AA. Mycotoxin Res, 2021, 37(1):97-103
[4] Pillay Y, Nagiah S, Chuturgoon AA. Toxicon, 2022, 210, 58-65
[5] Pillay Y, Nagiah S, Chuturgoon AA. Toxins, 2023, 15(4), 244
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Real-Time Monitoring Organic Reactions: Mechanistic Analysis of Reaction Intermediates/Species Using Online Mass Spectrometer

Akhilesh Kumar Verma

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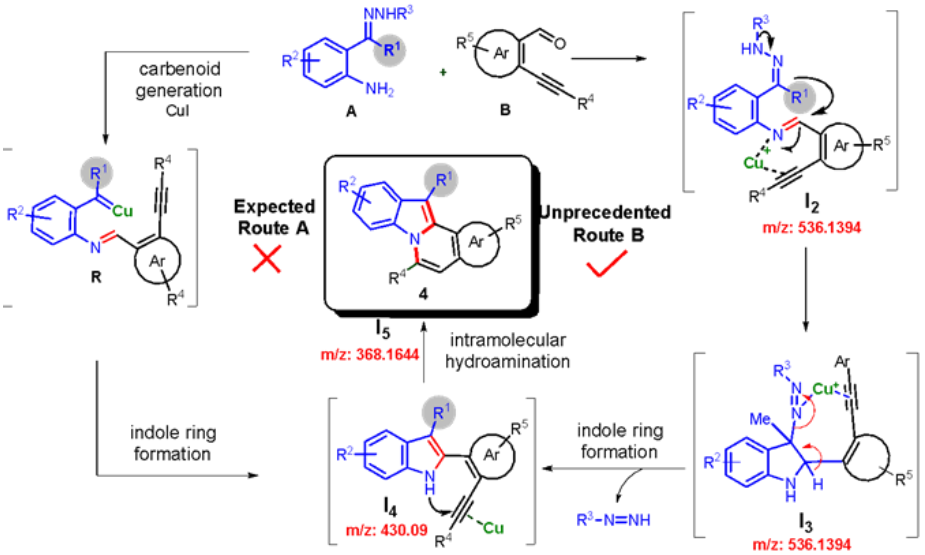
Abstract

In the past, a plethora of organic reactions have been discovered; however, most of these reaction reports proposed mechanistic pathways; finding the exact mechanism and reaction intermediate/short-lived intermediates is still challenging and unanswered. After the invention of LC/MS, it has become the technique of choice for online reaction monitoring. Online mass spectrometry is an underutilized tool in mechanistic organic chemistry despite its remarkable sensitivity and specificity to detect chemical species from a crude mixture. In this presentation, I would like to discuss some results from our laboratory in this direction.



 ISBN: 978-93-95033-37-4

Targeting A Unique mRNA Decapping Enzyme For Trypanosomatid Infectious Disease Drug Discovery

Maria Grechnikova[1], Paula Castaneda Londono[2], Leticia Pereira[2], Natalia Karolak[3], Marcin Warmiński [4], Marcelina Bednarczyk [4,5], Jacek Jemielity[5], Joanna Kowalska[4], Maria Gorna [3], Susanne Kramer[2] and Martin Zoltner[1]

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[2]Biocenter, University of Würzburg, Würzburg, Germany.
[3]Structural Biology Group, Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Warsaw, Poland
[4]Division of Biophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[5]Centre of New Technologies, University of Warsaw, Warsaw, Poland

Abstract

Trypanosomatids encode no homologues of canonical decapping enzymes, but employ the ApaH-like phosphatase ALPH1, belonging to a phosphatase family absent in mammalian systems, for the essential process of mRNA decapping. We have shown that *T. brucei* ALPH1 functions within a decapping complex composed of the trypanosome 5'-3'exoribonuclease Xrn1 ortholog XRNA and four proteins unique to Kinetoplastida. Based on the thorough characterisation of ALPH1, both biochemically and in the cellular context, we conclude that ALPH1 is meeting key criteria of a robust drug target. We set out to conduct a screening campaign to identify inhibitors with the potential to become highly selective candidate drugs for trypanosomatid caused diseases, including African sleeping sickness, Chagas Disease and leishmaniases. We have developed a robust luminescent assay to monitor ALPH1 activity for high throughput screening of inhibitors, relying on the quantification of ADP liberated from a dinucleotide cap analog by a coupled enzymatic assay. Specifically, liberated ADP is first converted into ATP by pyruvate kinase, fuelling the generation of a luminescent signal by luciferin/luciferase. Inhibitors identified in primary screens are tested for interference with ADP detection by a direct assay of ALPH1 decapping activity, to rule out false positives from inhibition of the coupled enzymatic reaction. This secondary screen relies on a m 7 GTP-pyrene probe, which readily yields fluorescence upon ALPH1 cleavage. We present data on the discovery of a unique mRNA decapping complex in trypanosomes, ALPH1 assay development and our target-based screening approach.

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Palladium-Catalyzed Regiodivergent C-H Olefination of Imidazo[1,2a] pyridine Carboxamide and Unactivated Alkenes

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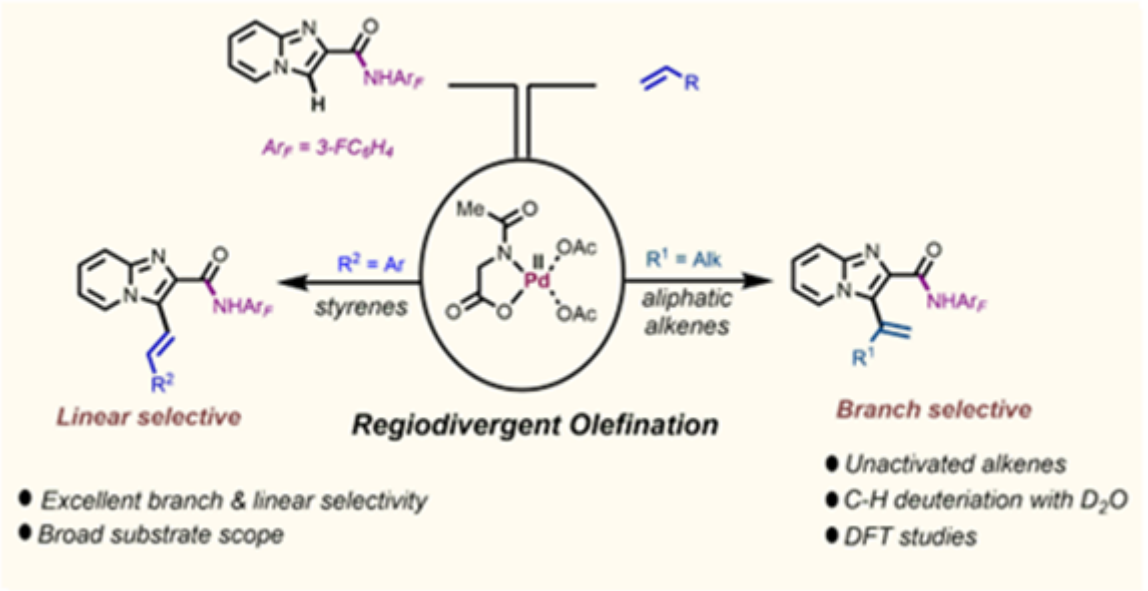
Abstract

In the last two decades, transition metal-catalyzed oxidative C-H alkenylation reactions via C-H bond activation have advanced significantly and led to many groundbreaking discoveries 1,2 . However, site selectivity and cleaving strong C-H bonds remain challenges. A ligand and directing group (DG) combination has allowed for site-selective C-H bond cleavage. Regiodivergent C-H olefination with a single catalytic system remains underdeveloped. Recently, a unified protocol was reported for Imidazo[1,2a] pyridine carboxamides, generating branched and linear olefinated products. The protocol can be applied for C-H deuteriation and is compatible with various styrenes and aliphatic alkenes. Preliminary experimental studies and computational investigations suggested that regiodivergent olefination can be controlled by olefin insertion and -hydride elimination steps.



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Modulating Intrinsic Behaviour of the Flavin Core for Biological Applications

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Abstract

Bioinspiration remains the driving force for various novel synthetic design offering fine tuning the key structural component for desired practical applications. In this context, naturally occurring flavin entity-, have been reported to play key role in numerous biological phenomenon involving electron transfer processes and luminescence.[1] For instance, flavin-based fluorescent proteins (FbFPs) has recently been reported to have advantage over the green fluorescent proteins due to their fluorescent capability in hypoxia conditions.[2] Considering the involvement of core flavin unit in various biological phenomenon, numerous synthetic model has been designed and tested for various chemical transformations and sensing applications.[3] While naturally the functional behavior is regulated via interaction with the apoprotein matrix, the suitable appendage need to be covalently linked to the flavin unit to modulate the key functional outcome. Herein, in this talk, we would like to discuss the subtle chemical modification around the core structural skeleton for biological applications. Focus of this talk will be to fine tune the photophysical/selective targeting properties of the flavin model for bioimaging and related applications.[4]

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Glycopeptide Antibiotic Derivatives Against Viruses

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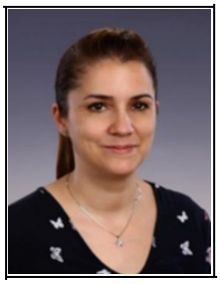

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Abstract

Glycopeptide antibiotics are used in the case of serious infections caused by Gram-positive bacteria including methicillin-resistant *Staphylococcus aureus* and *Enterococcus faecalis*. Teicoplanin and other lipoglycopeptides and some of their derivatives have antiviral activity as well. They were found to prevent the host cell entry process of Ebola virus, Middle East respiratory syndrome coronavirus (MERS-CoV), and severe acute respiratory syndrome coronavirus (SARS-CoV) by inhibiting the activity of the human Cathepsin L enzyme [1] while vancomycin with no lipophilic group has no antiviral activity. Teicoplanin was also proved to inhibit the viral 3CLPro main protease enzyme of SARS-CoV-2. As we also have experienced, the lipophilic side chain of the aforementioned glycopeptide antibiotics and their derivatives have important role in the antiviral activity, we proved that teicoplanin pseudoaglycone in the lack of lipophilic chain has no antiviral activity. We have synthesized different types of teicoplanin pseudoaglycone derivatives equipped with e.g. lipophilic octyl groups, lipophilic apocarotenoid side chains [2] and perfluorinated side chains with both lipophobic and hydrophobic properties [3]. Anti-influenza, -SARS-CoV-2 and other antiviral activity of the derivatives were determined, and in the case of SARS-CoV-2, the mode of action was examined by viral and human enzyme inhibitory tests.

Acknowledgement
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Current Trends in Natural Antibiotic Discovery

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Abstract

Natural antibiotics remain an important basis for clinical drug development. Moreover, the worldwide spread of resistant pathogens creates an urgent need for novel scaffolds with original modes of action. Nonetheless, both the discovery and the introduction of natural compounds into the clinic are hampered by a number of factors.

From the industrial point of view commercialization of new antimicrobials is severely delayed and implies no sustainable revenues. Compared with other therapeutic areas, antibiotics have similar R&D costs and failure rates, but only a fraction of the revenue prospects [1]. These fundamental problems lead to a low investment rate in the area and further exacerbate the lack of innovations.

From a scientific point of view, natural sources are still a very attractive source of active metabolites with valuable pharmacological properties. In the past few decades, the rate of discovery of novel antibiotics using the standard discovery platform, introduced by Selman Waksman at the beginning of the 20th century, has gradually reduced. Currently, there is a number of modern and emerging trends in the screening and identification of natural bioactive compounds [2]. The methods in this multisciplinary area can be divided into three groups: based on microbiology (e.g. *in situ* cultivation and microfluidics), chemistry (e.g. dereplication and MS-networking) and molecular biology (e.g metagenomics and mechanism-revealing reporter strains) [2].

Currently, the understanding of the molecular mode of action of natural products plays a crucial role. First of all, even compounds with no actual clinical perspectives can serve as a source of novel attractive targets for inhibiting the growth of resistant bacteria. Moreover, detailed information on the mechanisms of action and cytotoxicity is necessary for the development of semi-synthetic derivatives. In the case of bioactive compounds, even the slightest structural differences can bring dramatic changes to biological activity. For example, our recent studies on the tetracenomycin antibiotic family revealed that hydroxylation of the core can totally prevent cell entry [3], whether O^4-methylation abolishes ribosome binding ability [4]. Finally, natural componds can still be the source of novel drugs with intriguining biological activity. Recently we isolated a novel family of peptide antibiotics, named gausemycins, with striking structural novelty and an original membrane-assosiated antibacterial activity mechanism [5].

This work was supported by the Russian Science Foundation, project no. 23-24-00409, https://rscf.ru/en/project/23-24-00409/.

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Immunobiology of Long COVID-19 Syndrome

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Abstract

COVID−19 is caused by severe acute respiratory syndrome coronavirus 2 (SARS−CoV−2). Ongoing transmission of COVID-19 will add to the already existing cases with long COVID−19 syndrome posing a significant threat to public health. An estimated 87% of recovered patients have persistence of at least one symptom 60 days after acute disease; with over 10% of all COVID-19 patients manifesting long COVID. COVID-19 has claimed more than 1 million lives in the U.S. alone and more than 5,000 Americans have died from long COVID to date. Long COVID is a protean disorder and affected individuals manifest symptoms of nearly every organ system. Perhaps the most pressing public health crisis of long COVID- which has been estimated to cost the US healthcare system over $2 trillion- is the spectrum of neuropsychiatric illness. Patients recovered from acute COVID-19 disease are experiencing a variety of syndromes including post−traumatic stress disorder (PTSD), psychosis, anxiety, depression, insomnia, and obsessive−compulsive symptoms. Chronic stress associated with fear of illness, future uncertainty, traumatic memories, and social isolation increases the risk of a systemic pro-inflammatory state. The rate of new−onset neurological or psychiatric disorders in the 6 months following COVID−19 is 13% . A recent study described an increased risk of psychotic disorder, cognitive deficit, dementia, and epilepsy following SARS−CoV−2 infection relative to other respiratory illnesses. Hypotheses regarding causation invoke 3 broad etiologies: viral persistence, microvascular thrombosis, and protracted states of inflammation . Studies show the impact of viral invasion, inflammation, ischemic effects, and social and environmental factors in psychiatric illnesses, while data are lacking regarding the association of circulating biomarkers with new onset neuropsychiatric symptoms.

In this session, we will review current theories about the immunobiology of long COVID-19, with a focus on mechanisms of persistent disease. We will review new research approaches that focus on (1) identifying circulating inflammatory biomarkers (2) elucidating disorders of inflammation at the transcription level (3) determining the level of activation of inflammasomes, (4) identifying pro−thrombotic and metabolomic factors (5) assessing the role of variation in the genes known to be critical for neuropsychological functions (6) building predictive models to identify biomarker(s) signatures that can prognosticate neuropsychiatric outcomes.

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Artificial Intelligence Will Change Humanity Forever: Proactive Health Solutions For Disease Prevention

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Abstract

What are we witnessing today?

Today we are observing a specific change in society occurring as bold as the industrial revolution and impactful and dangerous as the atomic bomb: artificial intelligence, or AI. Through exponentially growing uses, applications, models and AI-related technologies (e.g., NVIDIA GPUs and quantum computing), we are on the cusp of seeing vast changes in societal infrastructure, social hierarchy and critically, biomedical advancements for disease control and public health. Many diseases are nearly impossible to treat due to the overwhelmingly complex nature of the interlocking pathways, genetic complexities, and number of combinations and permutations for proteins and nucleic acids as therapeutic targets for new drug agents. Overall, we still need humans to build these new vast architectures of scientific paradigm-changing modalities. These modes will embed AI into existing systems to rethink how we do what we do and reinvent new ways to tackle those problems more efficiently, and with better return on investment. For drug design, we face a significant challenge related to the sheer number of possible synthetic compounds with chemical space considered to be 'druglike' that can be screened against a host of human targets, that hardly scratches the surface of the vast number of interconnected relationships among all these targets acting as a unified machine.

Using AI to make a Toolkit Needed to Develop Proactive Health Solutions:

Step 1: Deduce the way to find optimal binders to modulate specific targets in a pathway.
Step 2: Find ways to control the flow upstream and downstream of these targets with consideration of all interacting partners.
Step 3: Predict outcomes due to genetic variance for precision-guided individualized medicine.
Step 4: Quality control the AI to determine what works and what does not – (i.e., fine tuning).
Step 5: make AI "bots" or "transformers of transformers" to complete complicated procedures for tackling problems from initiation to completion with minimal human intervention (long term goal).

Take home message:

To discover new therapeutics for humans we must take the state of the art and subsequently let existing and new AI methods train on this data store in large-scale experiments with massive amounts of data, storage and speed. Only then can we move from these early days of "first or second generation" AI to 3rd wave approaches that will enable wide-reaching public health initiatives that proactively "treat" individuals with underlying genetics or epigenetics ("ticking timebombs") in order to be healthy for their entire trajectory of lifespan. Proactive health solutions to prevent diseases will reduce morbidity, mortality and have significant economic savings.

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Youth Mental Health: Imagining safer and enabling spaces for young people

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Abstract

It is normal for youth to experience various types of emotional distress as they develop and mature. Most of the problems faced during this development phase are transient in nature. When symptoms persist, it may be time to seek professional assistance. While most youth are healthy, physically and emotionally, one in every four to five youth in the general population meet criteria for a lifetime mental disorder and as a result may face discrimination and negative attitudes. As with physical health, mental health is not merely the absence of disease or a mental health disorder. It includes emotional well-being, psychological well-being, social well-being and involves being able to successfully navigate the complexities of life, develop fulfilling relationships, adapt to change, utilise appropriate coping mechanisms to achieve well-being without discrimination. realise their potential, have their needs met, and develop skills that help them navigate the different environments they inhabit. The presence or absence of various combinations of protective and risk factors contribute to the mental health of youth and efforts can be undertaken to promote positive mental health and prevent or minimise mental health problems. Youth with mental health disorders may face challenges in their homes, school, community, and interpersonal relationships. Despite these challenges, for most youth, mental health distress is episodic, not permanent, and most can successfully navigate the challenges that come from experiencing a mental health disorder with treatment, peer and professional supports and services, and a strong family and social support network. Translation research in mental health can involve applying findings on basic behavioural processes and science relevant to changing human behaviour to develop and test more effective prevention programs and health education, as well as improving healthcare access, healthcare delivery, and individual health behaviours. A wealth of social and behavioural science on health behaviours, health decision making, and behavioural change can be applied to make community programs more effective. The presentation discusses how educational institutes and organisations involving youth can make a policy change and reimagine spaces for young people to make healthier and happier capital for the nation.

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Unveiling the Importance of Nontuberculous Mycobacteria as Potential Human Pathogens

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Abstract

Nontuberculous mycobacteria (NTM) are ubiquitous pathogens that had long being disregarded as potential human pathogens, especially in regions where tuberculosis (TB) is widespread. Infections caused by NTM have become a public health concern in recent decades, contributing significantly to clinical and economic burden worldwide. Of the more than 200 species of NTM identified so far, a large majority is not pathogenic to man and animals. However, these opportunistic pathogens may cause disease in subjects with predisposing conditions or compromised immunity. Though the diagnosis of NTM infection is difficult and time-consuming, technological advances and better awareness of the organisms have aided in diagnosing NTM disease in recent years. The prevalence of NTMs has significant geographic variations that might occur even within the same country. Common causative organisms of pulmonary infection are the slowly growing mycobacteria such as *Mycobacterium avium* complex and *Mycobacterium kansasii* and the rapidly growing mycobacteria, including *Mycobacterium abscessus* complex. Challenging diagnostic criteria and treatment options make it difficult to manage NTM disease. Hence, the awareness of diagnostic criteria and individual patient risk factors have a pivoting role in effective management of NTM infections. Improved NTM identification through quality-controlled diagnostic assays and clinico-laboratory coordination shall provide necessary epidemiological data to assess the importance and relevance of these isolates that were collectively dismissed up till recently as environmental contaminants.

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Metal-free Synthesis of Natural Product Inspired Glycohydrids as Anticancer Agents

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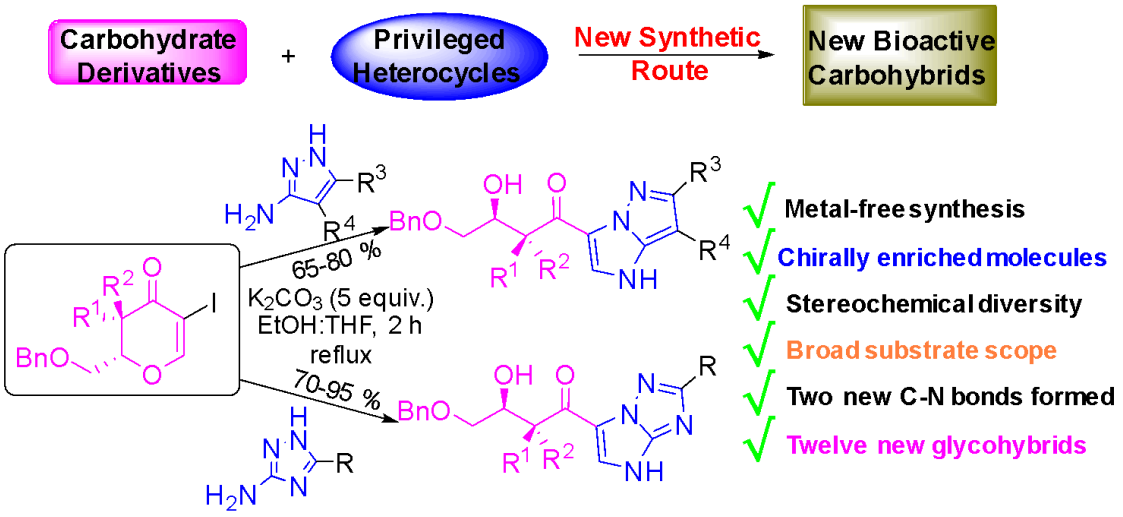
Abstract

Construction of drug like molecules is a challenging task in drug discovery process. imidazo-pyrazole and imidazo-triazole skeleton have gained larger attention among synthetic and medicinal chemists as they possess good biological and pharmacological properties. We aim to incorporate these bioactive scaffolds with carbohydrate adopting developed efficient synthetic protocol to synthesize new class of imidazo-pyrazole and imidazo-triazole glycohybrid molecules.[1] We have recently design and develop the synthesis of natural product-inspired naphthoquinone based glycohybrids.[2] We have also developed a new route for the preparation of an important chirally enriched and synthon Perlin's aldehyde.[3] The details of these findings will be presented therein.



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Indigenous Knowledge of Healing Among the Tribes

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Abstract

Indigenous knowledge implies inter-generational passed-on understanding and skills developed by the communities. It conventionally has a long temporal history and spatial association. The vertical transfer of Indigenous knowledge from one generation to another generation doesn't imply that it is unconditionally static rather it is dynamic in a way because the knowledge modifies itself as a response to change or transition in community lifestyle and environment. However, previous writings on indigenous knowledge of healing have mostly perceived it as unconditionally static knowledge and discussed it as heritage, searching for its recognition, protecting its threatened status, and arguing for its validity against the western framework. The indigenous approach to healing (IAH) is one such example of Indigenous knowledge and it is discussed as a kind of knowledge system, which consists of a set of common values, beliefs, worldviews, experiences and practices. It comprises lived, experiential and enacted knowledge and its determinants are mind, body, spirit, ecology and socio-cultural practices. IAH is constituted locally and embedded in the practices, institutions, relations and rituals. Unfortunately, most of the writings (on IAH) were also baffled by the misconception and false labelling of IAH (by empiricist framework) and set the motion rolling for validating IAH through the Western scientific or empiricist framework. This article attempts to investigate the indigenous concept of health and healing, Based on references from selected tribal communities, and also tries to find out if Is there any philosophical concept of indigenous healing etc.

***Keywords*:** Indigenous Knowledge, Healing, Tribes, Indigenous people

Antiviral Discovery Against Emerging Viruses

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Abstract

The world has witnessed the emergence and reemergence of several diseases in the last decades. Most of them are of viral origin, such as chikungunya, Zika, dengue, and SARS-CoV-2. For many of these viruses, there are no antivirals available for prophylaxis or treatment. Thus, the discovery and development of antivirals is of utmost importance. Here, we will discuss the challenges in antiviral drug research and how our Virology team in Brazil have partnered with chemists in Brazil, India, and South Africa to discovery potent antivirals against these important pathogens.

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The Multifunctional Autophagy Pathway as a Potential Drug Target for Malaria

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Abstract

Plasmodium parasites have a complex life cycle that transitions between mosquito and mammalian hosts and undergo continuous cellular remodeling to adapt to various drastic environments. Following hepatocyte invasion, the parasite discards superfluous organelles for intracellular replication, and the remnant organelles undergo extensive branching and mature into hepatic merozoites. Autophagy is a ubiquitous eukaryotic process that permits the recycling of intracellular components. During macroautophagy, the Atg8 protein is conjugated to phosphatidylethanolamine (PE) in autophagic membranes. In Apicomplexan parasites, two cysteine proteases, Atg4 and ovarian tumor unit (Otu), have been identified to delipidate Atg8 to release this protein from membranes. We investigated the role of cysteine proteases in Atg8 conjugation and deconjugation and found that the Plasmodium parasite consists of both activities. We successfully disrupted the genes Atg4 and Otu individually; however, simultaneously, they were refractory to deletion and essential for parasite survival. We found that Atg4 KO sporozoites invade and normally develop into early liver stages. However, nuclear and organelle differentiation was severely hampered during late stages and failed to mature into hepatic merozoites. We found a higher level of Atg8 in Atg4 KO parasites, and the deconjugation of Atg8 was hampered. We confirmed Otu localization on the apicoplast; however, parasites lacking Otu showed no visible developmental defects. Next, we show that the P. berghei autophagy-related E1-like enzyme Atg7 is expressed in the blood and liver stages, localized to the parasite cytosol and is essential for the localization of Atg8 on the membrane and the development of parasite blood and liver forms. We found that depleting Atg7 abolishes exocytosis of micronemes, organelle biogenesis and the formation of merozoites during liver stage development. Furthermore, we identified the compounds from the Maybridge library with a high docking score against PfAtg7. We show that these compounds inhibit apicoplast biogenesis and parasite development in both blood and liver stages. Overall, this study establishes the essential functions of Atg7 in Plasmodium blood and liver stages and highlights the potential of using it as a drug target against malaria.

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Antiparasitic Action of Mitochondrially Targeted Lipid Derivatives

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Abstract

Parasitic protozoa are among the most important eukaryotic targets for drug discovery. Due to metabolic adaptations, the mitochondria of these organisms represent a highly promising target for the design of new therapeutics. Indeed, in our recent work we have identified two novel promising anticancer compounds, mitochondrially targeted tamoxifen (MitoTam) and mitochondrial iron chelator (MitoDFO), as candidates for repurposing as antiparasitic agents with high selectivity **[1,2]**. Both compounds consist of a pharmacophore coupled to a charged triphosphonium group(s) *via* a linear alkyl linker. They exhibit high selectivity against a range of pathogens, including *Plasmodium falciparum* and several species of trypanosomatid parasites, and are effective against intracellular *Leishmania* infection. MitoTam treatment was also effective *in vivo* and significantly reduced parasitemia of *Leishmania mexicana* and *Trypanosoma brucei* in their respective animal infection models. Biochemical experiments suggest that part of the mode of action of both compounds is a direct effect on the integrity of the inner mitochondrial membrane and, surprisingly, the antiparasitic effect is only partially dependent on the presence of the pharmacophore, indicating the activity of the vector molecule itself. Our current research focuses on the *in vitro* screening of a library of novel synthetic unnatural anti-parasitic mitochondrially targeted lipids and the determination of their mechanisms of action, using *Trypanosoma brucei* as a well-established model to study mitochondrial processes, with the ultimate goal of designing optimal structures with maximum selectivity over mammalian cells and enhanced inhibitory activity against important human pathogens.

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Carbohydrate-Based Small Molecules Derivatives: Stay on the Roads Towards Bioactive Compounds

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Abstract

Organic Synthesis is an area of basic research and one of the pillars in the development of new drugs, and the discovery of New Chemical Entities with biological applications has been a promising path for synthetic organic chemists. Recently, we have been exploring the construction of carbohydrate-based small molecule derivatives bearing 1,4-naphthoquinone and azo-heterocycles moieties, which were synthesized using protection/deprotection/glycosylation/epoxidation/cyclization protocols. [1-4] This portfolio of compounds was then evaluated against several diseases, such as tuberculosis, [3] viruses (Zika, [4,5] SARS-CoV-2 [5]), and cancer. [5] These results indicate a few of leading candidates for future clinical trials.

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Regioselective Chalcogenation of Quinoxolinones and Benzoxazines *via* C-H activation

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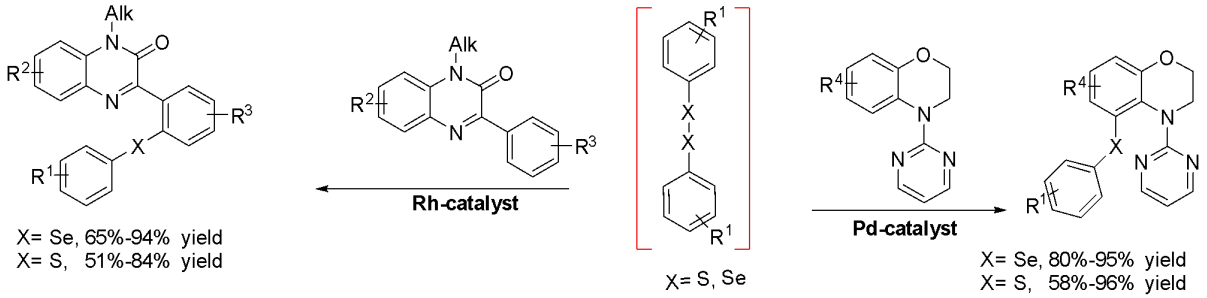
Abstract



In continuous pursuit to develop newer methodology for synthesis of bioactive molecules, we have developed green and sustainable methodologies for the regioselective direct C-H chalcogenation of quinoxolinones and benzoxazines using Rhodium and Palladium as catalyst. Metal-directing property of the nitrogen atom has been exploited for the synthesis of bioactive compounds. Several control experiments and Kinetic studies have also been performed in order to establish the mechanism. A wide variety of diphenyl disulphiles, diphenyl diselenides were exposed to these newly developed methodologies and all of them have delivered the chalcogenated products in excellent yields. Detail of this chemistry would be discussed during the talk.

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Current Trends in Photosensitizing Antiviral Drugs

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Abstract

The last decade has been marked by great advances in antiviral drug development. However, despite significant progress in the treatment of viral diseases, the global COVID-19 pandemic caused by the SARS-CoV-2 coronavirus showed that the humanity is not ready for further challenges from new, previously poorly studied diseases. In this regard, the development of universal antiviral drugs with a broad spectrum of action becomes especially relevant.

Amphipathic photosensitizers already demonstrate excellent antiviral activity on enveloped viruses, such as herpes simplex virus (HSV), tick-borne encephalitis virus (TBEV) and many others [1]. The action of such substances is based on the generation of singlet oxygen, which damages the viral membrane and inhibits its fusion with the membrane of a healthy cell [2]. To interact with the membrane as effectively as possible, a photosensitizer should contain two main parts: a nonpolar aromatic core capable of generating singlet oxygen and a polar group located on a long linker for stronger attachment to the membrane [3]. The location of the photosensitizing chromophore in the lipid bilayer is crucially important for antiviral activity [4].

Derivatives of the pentacyclic aromatic hydrocarbon perylene demonstrate high activity against enveloped viruses [5,6], but low solubility in aqueous media severely limits their use. At present, active development of drugs based on other photogenerating nuclei, such as BODIPY and cyanines, is underway.

One of the main problems with existing photosensitizing antiviral drugs is the need to excite themwith visible light. Thus, they can be used to treat surface viruses, but light does not penetrate intothe body. To solve this problem, the development of photosensitizing dyes that absorb in the near-infrared range is underway. Infrared light is part of the phototherapeutic window, where light is able to pass through tissues and excite the dye even inside the body [7].

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Synthesis of Various Functionalized Aza Heterocycles from Aryl Methyl Ketones of Biological Importance

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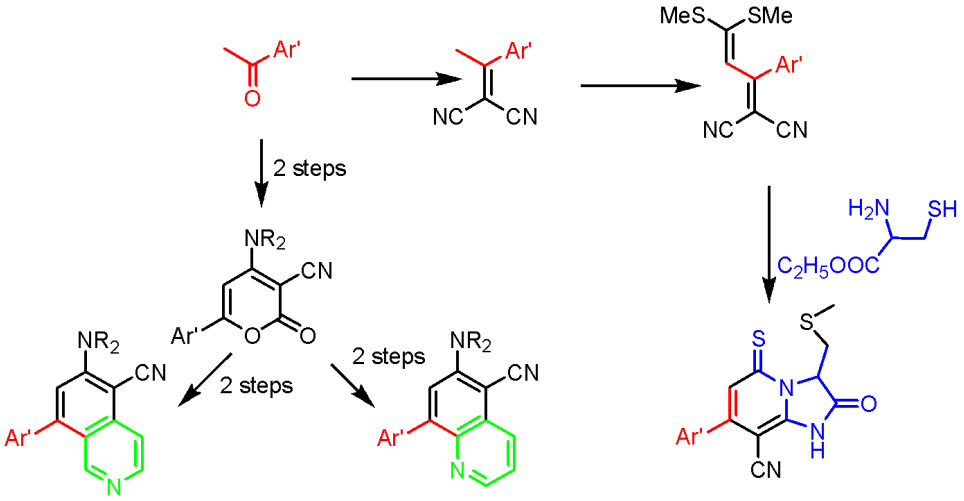
Abstract



Aryl methyl ketones are very well known primary precursor for the synthesis of a large class of molecules. Our group is involved in using ketone for the synthesis of various ketene dithioacetals and pyran and to explore further chemistry.[1] Imidazopyridines are interesting heterocyclic compounds containing two fused heterocyclic motifs, i.e., pyridine and imidazole, in one molecule. we have developed a cascade one-pot methodology to synthesize Imidazopyridines using 1,6-Michael acceptor ketene dithioacetals under mild conditions. we also reported iodine and DMSO-promoted synthesis of multifunctional quinolines and isoquinolines using 6-aryl-4-*sec*.amino-2-oxo-2*H*-pyran-3-carbonitriles and 1-Boc-4-piperidone/1-Boc-3-piperidone as precursors. Synthesis of N-Boc-1,2,3,4-tetrahydroisoquinoline was carried out by ring transformation of suitably functionalized 2-pyranones with 1-Boc-4-piperidone in DMSO under basic conditions. The N-Boc-1,2,3,4-tetrahydroisoquinoline crude was obtained and treated with iodine and DMSO to afford the desired isoquinoline. Using iodine and DMSO, consecutive two-step Boc deprotection and aromatization of isoquinolines occur. The reaction proceeded efficiently, and the desired isoquinolines were achieved in good yields. The generality of the protocol was tested by using various functionalized 2-pyranones with 1-Boc-4-piperidone. Earlier we have achieved a one-pot approach for the synthesis of benzo[h]quimolines[2] and now new azaheterocycles were established ketene dithioacetals.[3]

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Synthesis of Fluorine Containing Cannabinoid Derivatives with Various Biological Activities

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Abstract

Cannabidiol (CBD) and cannabigerol (CBG) are non-psychotropic phytocannabinoids that can be found in *Cannabis sativa*. Unlike tetrahydrocannabinol (THC), they cannot alter the consciousness. It is known that phytocannabinoids interact with cannabinoid receptors (CB1 and CB2) and they have several other molecular targets in the human body. Many different beneficial pharmacological effects are attributed to them which are intensively examined. The production and biological investigation of semi-synthetic cannabinoid derivatives are getting more and more popular but there are only a few examples of systematic synthetic modifications in the scientific literature [1-4].

Previously, in our research group, CBD and CBG derivatives containing amino groups were successfully synthesized from amines and cannabinoids by Mannich-type reaction [4]. As a continuation of this research, we used fluorinated compounds containing amino groups for the Mannich-type reactions of CBD and CBG. By using various simple mono-, di- and trifluoroamines, in the presence of formaldehyde, we have successfully synthesized mono- and disubstituted compounds containing one or two oxazine rings with fluorinated substituents. The anti-SARS-CoV-2 activity and the antibacterial effect of the synthesized derivatives were studied by collaborating partners. Some of these compounds had weak antibacterial and moderate antiviral activity. The examination of antiproliferative and antioxidant effects are under process.

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Recent update on antimalarials; Parasite proteases are potential target

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Abstract

The family of apicomplexan specific proteins contains caspases–like proteases called "Metacaspases". These enzymes are present in the malaria parasite but absent in human; therefore, these enzymes can be explored as potential drug targets. We deleted this enzyme from parasite using a gene knockout strategy to decipher its precise function. This study has identified that Metacaspase plays an important role in parasite transmission since it is critical for the formation of gametocytes, and for maintaining an appropriate number of infectious sporozoites required for sporogony. It is noticeable that a significant reduction in gametocyte, oocysts, ookinete and sporozoites load along with a delay in hepatocytes invasion were observed in the knockout parasite. Furthermore, this study found the two Metacaspase inhibitory molecules known as C-532 and C-533, which specifically inhibited the enzyme activity, abolished the in vitro parasite growth, and also impaired the transmission cycle of *P. falciparum* and *P. berghei* in An. stephensi. Our findings suggested that C-532 and C-533 critically affected the malaria transmission biology, and could be explored as potential compounds in a large scale of animal trial.

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HEA (HydroxyEthylAmine) Based Potent And Safe Anti-Malarials

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Abstract

Emerging resistance of the front-line antimalarials towards the malaria parasite, *Plasmodium falciparum* (*Pf*), and the paucity of novel effective drugs are together are the roadblocks against malaria eradication initiatives, and hence a burden to the human health.

In the past, antiplasmodial activities of hydroxyethylamine (HEA) analogs have been extensively investigated, and recently it emerged as crucial pharmacophore to achieve potent multistage antimalarials. Development of novel structurally unique compounds centered at validated pharmacophore remains one of the important strategies to identify novel drug molecules. While keeping the HEA, we diversified the side chain to improve the solubility and permeability.

Hydroxyethylamine (HEA)-based novel compounds were synthesized (LTC-1084 to LTC 1089) and their activity against *Plasmodium falciparum* 3D7 was assessed, identifying a few hits without any apparent toxicity. Hits LTC 1084, LTC 1085 and LTC 1089 exhibited activity against Pf 3D7 (IC50 =0.55, 0.23 and 0.4 uM respectively). The selectivity index or therpeutic index was greater than 1000 for LTC 1084(=1161), LTC 1085 (=1391) and 100 for LTC 1089.

In a RBC lysis assay these compouds did not show any significant lysis upto 100 uM. Thus indicating a safe profile. These compound were found to be slow acting and maximum inhibition was observed at 72 post treatment in a ring survival assay. Treated parasites were mostly present in trophozoite stage at 48 hour post treatment. Parasites were not able to mature into the schizonts. Further work to test in invivo is under progress.

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Ethno Medicinal Alternatives in Regenerative Pharmacology: A Talismanic Tool to Wound Healing

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Abstract

Regenerative medicine has evolved in modern days with the advent of biomedical research to combat the challenges of scar free and fast healing in human as well as animal subjects. Ayurveda, an ancient treatise also mentioned the term Varna for wound injury. Wound healing is proclaimed as a complex pathophysiological process that involves interplay between several immune cells and cytokine and chemokines mediators *vis a vis* several growth factors viz. vascular endothelial growth factor (VEGF), Transforming growth factorβ (TGFβ) etc. (Singer and Clark, 1999). Three overlapping phases viz. hemostasis and inflammatory phase, proliferation phase and tissue remodeling, characterize the course of normal healing. Several health benefits of goat milk and its associated products are scientifically proven. Goat milk has anti-inflammatory, antioxidant, antiviral, anticancerous and anti allergic activity etc. (Kao et al., 2020; Nayik et al., 2021). Kao et al. (2020) reported that goat milk could enhanced the adaptive and innate immunity and also alleviated the air way inflammation through triggering of several cytokines i.e. IL-6, IL-10, TNF-α and antibodies i.e. IgA, IgG and IgM etc. Goat milk has richness in caprylic acid and thus may be a potential biopharmaceutical agent in future for wound healing treatment. In the modern context of effective healing, it is quite essential to rethink the pharmacodynamics and therapeutic efficacy of natural sources against wounds.

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Synthesis of Fluorescent and Therapeutic Antibody Conjugates Using Various Site-Specific Approaches

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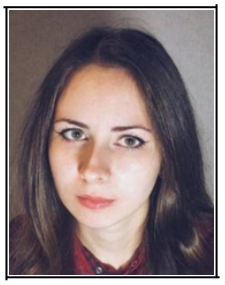

Abstract

An antibody-drug conjugate (ADC) is a monoclonal antibody covalently linked to a small molecule therapeutic (often antitumor) agent by means of a linker. The principle of action of conjugates is as follows: after selective binding of the antigenic part of the construct to some antigen on the surface of the tumor cell, the conjugate disintegrates (in lysosomes after internalization or in the extracellular matrix) with release of a cytotoxic drug leading to cell death.

ADCs are well established in the clinic. The FDA has approved twelve drugs for use on patients, and over a hundred more are in various stages of clinical trials [1].

The current trends in the design of antibody-drug conjugates are site-specific conjugation of antibody and linker-drug, homogeneity of the conjugate, and high toxicity of the therapeutic agent [1]. At the same time, the classical approaches to antibody modification used to synthesize all ADCs approved to date, namely modification by lysines and cysteines, do not result in site-specific conjugates. In our work, we use a periodate oxidation of glycanes with subsequent oxime ligation [2-5] or a two-step enzymatic approach [6], which consists of removing the Fc glycans of the antibody fragment and then ligating the target molecule using natural enzymes.

We use monomethylauristatin E (MMAE) as a cytotoxic payload conjugated to the antibody using linkers based on cyanine dyes and cleavable oligopeptide fragments. The conjugates are synthesized based on the well-known therapeutic antibody trastuzumab to the tumor antigen HER2 and the novel antibody 6H8 to the tumor-specific antigen PRAME.

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Engineered siRNA Coated Cs-AuNPs Leverages the Selective Knockdown of Osteoporotic Gene Sost and Promote Osteogenesis in an *in-vitro* Model

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Abstract

Aim: Osteoporosis is a bone-incapacitating malady characterised by bone mass loss and deterioration of bone microarchitecture. Current treatments for osteoporosis are limited by adverse effects and long-term safety issues. Osteoporosis being a systemic skeletal disorder is characterised by reduced osteoblast differentiation, predominantly by overexpression of the Sost gene. A layer-by-layer approach enabled encapsulation of Sost siRNA to enhance the short half-life and poor transfection capacity of siRNA.

Materials & methods: Polyethyleneimine and siRNA on chitosan-coated gold nanoparticles (PEI/siRNA/Cs-AuNPs) were engineered using chitosan-reduced gold nanoparticles. They were characterised by dynamic light scattering, scanning electron microscopy, transmission electron microscopy, Fourier transform infrared and gel-mobility assays. Detailed in vitro experiments, gene silencing and western blots were performed.

Results: A total of 80% knockdown of the target sclerostin protein was observed by PEI/siRNA/Cs-AuNPs, q-PCR showed threefold downregulation of the Sost gene. Osteogenic markers RunX2 and Alp were significantly upregulated.

Conclusion: We report a safe, biocompatible nanotherapeutic strategy to enhance siRNA protection and subsequent silencing to augment bone formation. Sclerostin protein is secreted by differentiated osteoblasts that is encoded by SOST gene; it decreases bone formation by reducing osteoblast differentiation through inhibition of the Wnt signaling pathway. Silencing the SOST gene using RNA interference (RNAi) could therefore be an effective way to treat osteoporosis. Here, we investigate the utility of PEI/siRNA/Cs-AuNPs and PPi/ siRNA/Cs-AuNPs formulations of siRNA to silence the SOST gene *in vitro* and for future use in *in vivo*.

Keywords: Osteoporosis, Gold-chitosan nanoparticles, Wnt signaling pathway, siRNA, SOST gene, Osteogenic biomarkers.

Upregulation of Energy Metabolism and pro-inflammatory Signaling Confers Radio-Protection in *in-vitro* and *in-vivo* Small Animal Models

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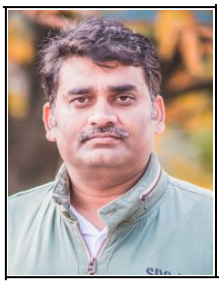

Abstract

Exposure to Ionizing radiation (IR) causes deleterious molecular events resulting in acute radiation syndrome and posing severe threat to human health and sometimes even lead to mortality. Preserving normal tissues from ionizing radiation (IR)-induced damage is imperative in nuclear incidents and radio-therapeutic applications. Therefore, there is a need to develop potent and safe radioprotective agents for radio-nuclear emergencies. A tight coupling between the metabolic status and signal transduction is critical for maintenance of homeostasis and recovery from radiation damage. One of the metabolic changes associated with the radio-resistance of cells is the upregulation of glucose metabolism and its inhibition results in radio-sensitization of resistant cells. Therefore, we induced glycolysis at cellular level using various pharmacological agents and cytokine Interleukin-6 (IL-6) to understand molecular mechanisms underlying radio-resistance linked to elevated glycolysis. We found that uncoupling of mitochondrial respiration using 2,4 dinitro phenol, inhibition of PTEN to activate Akt signaling and treatment of cells with IL-6 induces glucose consumption and lactate production. Enhanced metabolism intricately regulates cellular pathways involved in redox balance, maintenance of mitochondrial homeostasis, facilitated DNA repair, apoptosis, and survival during inflammatory responses, thereby safeguarding cells after radiation exposure. The experimental observations in *in-vitro* cellular models were also validated in *in-vivo* black mice model. Treatment of animals with these metabolic modifiers displayed enhanced recovery from radiation induced severe hematopoietic and GI acute radiation syndromes and protects from mortality.

These findings underscore the potential of metabolic modifiers as a candidate for the development of a radioprotector, offering the promise of ameliorating acute radiation syndromes and reducing radiation-induced mortality.

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BGP-15 Protects Against Doxorubicin-Induced Cell Toxicity Via Enhanced Mitochondrial Function

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Abstract

Doxorubicin (DOX) is a commonly used chemotherapeutic agent for the treatment of different solid and non-solid cancers. However, it does have limited application due to its remarkable cardiotoxicity. The mechanism of DOX-induced cardiotoxicity is still controversial. The major current theories include the production of reactive oxygen species (ROS), mitochondria dysfunction, apoptosis, and autophagy dysregulation [1].

Meanwhile, BGP-15 - a derivation of nicotinic amidoxime, is a new member of insulin sensitizer drug that was developed by Hungarian scientists - has been demonstrated with cardioprotective effects [2]. In our study, we investigated the BGP-15 effects on the DOX-exposed cardiomyocytes, whether the protective effects of BGP-15 pretreatment are predominantly via preserving mitochondrial function, reducing mitochondrial ROS production, and it has influence on autophagy processes. In order to, we performed cell viability tests (MTT and LDH assay), MitoSOX Red and JC-1 staining; moreover we measured apoptotic, and autophagic protein expression levels and autophagic markers localizations.

We found that BGP-15 pretreatment has significantly improved the cell viability after 12 and 24 hours DOX exposure. BGP-15 withheld the lactate dehydrogenase (LDH) release and decreased the cell apoptosis induced by DOX. Additionally, BGP-15 pretreatment attenuated the level of mitochondrial oxidative stress and the loss of mitochondrial membrane potential. Besides, BGP-15 further slightly modulated the autophagic flux which was measurably decreased by DOX treatment. Hence, our findings clearly revealed that BGP-15 might be a promising agent for alleviating the cardiotoxicity of DOX. In conclusion, our results indicated that BGP-15 could prevent DOX-induced cell toxicity by decreasing mitochondrial ROS production and attenuating mitochondrial depolarization.

This research was funded by the GINOP-2.3.4-15-2020-00008, TKP2021-EGA-18 and NKFI-143360 projects.

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Zinc Pyrithione Inhibits Blood Stage Parasites of *Plasmodium falciparum* in Culture

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Abstract

Over time, the malarial parasite *Plasmodium falciparum* has evolved resistance to a number of antimalarial drugs. Particularly in areas where the disease is endemic, clinical resistance is a significant obstacle to the efficient treatment and management of malaria. Drug repurposing is an alternative strategy for combating drug-resistant parasites. This study sought to determine an FDA approved microbicidal agent Zinc pyrithione (ZnPT), has any antiplasmodial effects on blood-stage parasites of *P. falciparum* chloroquine sensitive (*Pf*3D7) and resistant strain (*Pf*INDO). Based on the time-inhibition kinetics assay, the parasite viability was significantly inhibited by ZnPT treatment for 96 (0.68 µM and 0.37 µM) and 72 hours (0.63 µM and 0.61 µM), followed by 48h (0.75 µM and 2.20 µM) and moderate inhibitory effects for 12 and 24 hours in both *Pf*3D7 and *Pf*INDO culture. Stage-specific treatment revealed that ZnPT-exposed trophozoites and schizonts showed greater susceptibility than ring-stage parasites. Phenotypic assays displayed that trophozoites and schizonts failed to mature and exhibited aberrant morphologies, such as condensed nuclei by Giemsa staining. Furthermore, ZnPT in combination with dihydro-artemisinin and chloroquine demonstrated additive interaction in both *Pf*3D7 and *Pf* INDO parasites. At therapeutic dosages, ZnPT did not result in hemolysis of the host erythrocytes (uninfected). This is the first report to show that ZnPT is effective in blood stages of human *P. falciparum* in culture, having immense therapeutic potential as an antimalarial agent.

Keywords: *Plasmodium*, zinc pyrithione, drug-repurposing, time-kill kinetics, drug-combination

Catalyst-Controlled C–H Allylation and Annulation of (Hetero)arenes Using Cyclic Carbonates

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Abstract

Transition-metal-catalyzed C–H allylation reaction has led to prodigious attention as it is capable to expedite the introduction of allyl fragments into (hetero)aromatic frameworks beyond the conventional allylation reactions.[1] In this context, the directing group-assisted C–H allylation reaction has recognized as a valuable strategy because of the rapid and regioselective construction of allylarene scaffolds without tedious prefunctionalization.[2] To date, a number of allylating agents have been successfully studied under various transition-metal catalysis. The integration of C–H functionalization and tandem cyclization has emerged as a powerful approach for the construction of *N*-, *O*-, and *S*-heterocycles.[3] To execute this protocol, annulation modes involving the electrophilic addition of π-unsaturates or the nucleophilic addition of C–M intermediates into directing groups have been intensively investigated.

In continuation of our recent studies on the synthesis of biologically relevant heterocyclic molecules based on catalytic C−H functionalization, herein I will present the transition metal catalyzed synthesis of various *N*-Heterocycles and late-stage drug candidates.[4] These reactions were facilitated via in situ generated allylated hetero(arenes) from cyclic carbonates and subsequent intramolecular olefin insertion process. To gain mechanistic insight of this transformation, deuterium-labeling experiment was also performed.

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The Importance of Collaboration between Academia and Industry in Pharmaceutical R&D

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Abstract

Today, there is a strong focus on supporting health innovation at both national and international level. The development of new and innovative formulations is also part of the strategic plans of several academic sectors. However, this cannot be achieved effectively unless universities work closely with industry, thus strengthening the third mission of universities. In this way, international competitiveness can be significantly enhanced.

The methodology used is competence-based and focuses on the training of young researchers. Multidisciplinary research networks have been set up to implement the research direction agreed with industrial partners. We applied a comprehensive research and development competencies methodology that develops a model system for financial feasibility analysis that is aligned with self-sustaining research.

As a result of the new approach of the multidisciplinary research network and the cooperation between industry, the University of Debrecen has developed product and service-oriented research directions, which also focus on financial and social utility.

The network has learnt at the service level about quality-assured RDI activities ranging from laboratory-scale formulation development to university-sponsored human pilot studies. For implementation, we have set up a medium-scale manufacturing facility. As an achievement, we have also paid special attention to ensuring the next generation of young researchers. We have taught competence in an interdisciplinary approach to research. We have strengthened national and international networking competences by giving them the opportunity to develop their own network of contacts. We made sure that they recognised the benefits of active participation in research teams. We have reinforced the practice of examining research results in terms of patentability. the research network involved 11 research teams working together at different levels. We focused on in vitro and in vivo results and how they relate to each other, and the artificial intelligence team developed algorithms that the research results can be analyzed more efficiently.

As a result of the establishment of an efficient multidisciplinary research network, a spin-off company was founded together with industrial partners, and many new technologies and prototypes were developed. In order to increase the TRL level, we have prepared effective plans. As a result of successful cooperation between academia and industry, R&D activity in the health industry reached a new level, further strengthening the development and implementation of a new multidisciplinary research approach.

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Characterization of Plasmodium and Leishmania Calcium Channel: Potential Anti-Parasitic target

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Abstract

One of the greatest challenges in infectious disease research has been decreasing the morbidity and mortality associated with parasitic diseases. Despite making considerable progress in vector control and disease reduction efforts through awareness, mass spraying, and the use of insecticide-treated bed nets, malaria and leishmaniasis cases are still on the rise. Both diseases overlap in their prevalence due to the vectors (Mosquito and Sand fly) preferring the tropical temperature. Visceral leishmaniasis (VL), the most severe and fatal form of leishmaniasis caused by *Leishmania donovani*, is endemic in parts of India, Africa, and South-West Asia overlapping the malaria belt. Currently, the few anti-leishmanial drugs that are available have limitations due to serious side effects/toxicity, higher cost, and emergence of drug-resistant parasites. Additionally, there is a wide gap in their effectiveness on intracellular stages, i.e., amastigotes. Similarly, malaria control relies heavily on the administration of Artemisinin based combination therapies (ACTs) as the first-line of treatment. However, the rapid spread of ACT-and multi-drug resistant parasite in many parts of endemic regions, creating serious challenges. Therefore, there is an urgent need to discover novel anti-parasitic that are targeted at essential pathways of the parasite to circumvent development of resistance. To develop new therapeutics for both these parasites, we have utilized a multifaceted approach to discover and evaluate the target-specific hits from experimental, approved, natural, in-house synthetic drug libraries through computer-aided drug design (CAAD)/high-throughput virtual screening (HTVS) tools and State-of-art molecular testing methods. As such, we have embarked on expanding the understanding of mechanism of action of series of active leads, target structure characterization, developing new 3D structure, functional characterization of *L. donovani* and *P. falciparum* calcium (Ca^{2+}) channel protein, expand the target-based drug discovery pipeline. With this pipeline been functional, we now have a validated several lead compounds having high potency against *P. falciparum and L. donovani* specifically targeted at Ca^{2+} homeostasis (*Ld*PDK/*Ld*TRP and *Pf*TRP) due to similarity at the core binding structure. Collectively, we have successfully implemented our pipeline to facilitate SAR-based rational improvement of lead compounds through integration of cheminformatics, deduce new structure, target characterization by engineering Ca^{2+} sensor based high content (HC) imaging assays, and validation of anti-parasitic activities through HTS platform.

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Vaccine and diagnostic potential of early and late stage expressing protein antigens of *Mycobacterium tuberculosis*

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Abstract

Mycobacterium tuberculosis persists in latent stage for long period of time without causing disease. The active TB diseases express early stage antigens, ESAT6 and CFP10 whereas the latent TB stage expresses late stage specific antigens mainly DosR regulon. As BCG mainly express early stage antigens, we tested immunogenicity of four DosR regulon proteins namely, Rv2626c, Rv2627, Rv2628 and Rv2032 by performing T cell phenotyping studies, estimation of expression levels of transcription factors T-Bet and GATA-3 which determine the protective Th1 or regulatory Th2 type of response and cytokine analysis in PBMC of normal individuals, TB patients and their close contacts. These DosR proteins induced IFN-γ+ CD4 and IFN-γ+ CD8 T cells, memory T associated CD4+/CD45RO+and CD8+/CD45RO+T cells and cytokines like IFN-γ, IL-2, and IL-17 but not IL-4, IL-10, and TGF-β in both patients and contacts. The proteins stimulated expression of T-Bet transcription factor which is the master regulator for immune-protective TH1 response. Decrease in frequency of CD4/CD25/ FoxP3 regulatory T cells in response to these proteins further emphasized the importance of vaccine potential of these proteins. We further observed that these DosR antigens induced a higher proportion of T cells producing IFN-γ by PBMC from Latent TB compared to active TB patients and there was a differential expression of cytokines from these two types. The current immunodiagnostic test, IGRA, also employs early stage antigens. We propose that these late stage DosR antigens can be utilized for production of a multi-cytokine releasing assay to discriminate between LTBI and active TB.

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Discovery, Crystallographic Studies and Mechanistic Investigations of Phenylalanine Peptidomimetic Derivatives as Potent HIV Capsid Modulators

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Abstract

The multifunctional HIV-1 capsid protein (CA) represents a highly appealing target in HIV-1 medication research[1]. With PF74 as the lead compound, our previous efforts involved replacing the indole moiety with benzenesulfonamide piperazinone and obtained a novel HIV-1 CA modulator 11L[2]. Herein, the structure-based optimization of compound 11L to improve its antiviral activity and metabolic stability culminated in the identification of quinazolin-4-one-bearing phenylalanine derivatives. Notably, derivatives **12a2** and **21a2** showed significant improvements, with 2.5-fold over 11L and 7.3-fold over PF74 for HIV-1, and approximately 40-fold over PF74 for HIV-2. The X-ray co-crystal structures confirmed the multiple pocket occupation of **12a2** and **21a2** in the binding site. Mechanistic investigation studies demonstrated the compounds' antiviral activities featuring a dual-stage inhibition profile. At the early stage, these modulators seemed to disrupt the interactions between CA and host factors, and the late-stage activity might be facilitated by enhancing CA misassembly. Remarkably, **12a2** and **21a2** significantly promoted capsid misassembly, outperforming 11L, PF74, and LEN. The substitution of easily metabolized amide bond with quinoline-4-one marginally enhanced the stability of **12a2** in human liver microsomes compared to controls. In view of these merits, **12a2** and **21a2** underscores their potential as potent HIV CA modulators, thus paving the way for future advancements in anti-HIV drug design.

***Keywords**:* HIV-1; capsid modulator; crystallographic studies; mechanistic investigations

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PALs: High-Speed Precision Bio-Conjugation

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Abstract

Peptidyl Asx-specific ligases (PALs), discovered from cyclotide-producing plants, perform rapid site-specific peptide cyclization, cell-surface labelling, protein semi-synthesis and protein conjugation. In this regard, PALs are powerful and versatile tools for the generation of bioconjugates with applications in various disease areas including in cancer treatment and diagnosis. Radionuclide drug conjugates and antibody-drug conjugates made with PALs have improved in vivo properties, rendering them more efficacious and safer compared to those produced by conventional chemical methods. Details of these undertakings will be discussed.

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Exploration of Synthetic Strategies and Biological Assessment: Unveiling the Potential of Some Natural and Marine Natural Compounds of Medicinal Interest

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Abstract

"The need for efficient and practical synthesis of biologically active molecules remains one of the greatest intellectual challenges with which chemists are faced in the 21st Century".

Throughout the ages humans have relied on Nature to cater for their basic needs, not the least of which are medicines for the treatment of a wide spectrum of diseases [1]. The synthesis of complex natural products continues to occupy an important position in organic chemistry research, not only because nature provides us with some of the most synthetically challenging molecules that we can ever aspire to synthesize, but also because research in this area frequently drives important breakthroughs in methodology. Structurally complex, biologically active naturally occurring substances of marine origin continue to spur the interest of both chemists and biologists as they demonstrate antiviral, antimicrobial, anti-oxidant, and many more biological activities [2,3]. This is an important area to work on as the major challenge with the biologically active isolated natural products is their limited availability through natural resources and their isolation is very tedious and time consuming process [4]. Further, they are usually isolated in very small quantities, hindering further studies to establish their biological activities as well as structural modifications and their constant supply from natural sources is problematic or virtually impossible. In addition, chemoselective derivatization of marine natural products themselves is usually quite difficult because of their sensitive and elaborate molecular structures, and access to their structural analogs is severely restricted in many cases.

Therefore, chemical synthesis of natural and marine compounds in larger quantities and by sufficient means is necessary to investigate their biological implications and this strategic synthetic methodology is focused in our lab [5,6]. Further, considering significance of fluorine incorporation in heterocycles and taking an overview on their biological activities, synthesis of fluorinated analogues of some natural products is planned. An understanding of mechanism, coupled with knowledge of physicochemical properties affected by fluorine substitution has aided in rational drug design of many pharmaceutical agents. Design , strategic synthesis and significance of target molecules will be presented.

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Pharmacological Research of Newly Synthesized CBD Derivatives

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Abstract

Cannabidiol (CBD) is a non-psychotropic phytocannabinoid that can be found in Cannabis sativa, and it has been observed in the latest decades, since it has plenty of pharmacological effects. Some of these effects are useful in cardiovascular diseases, in which we have a high interest in our research group. Our colleagues in Department of Pharmaceutical Chemistry managed to prepare three CBD derivatives substituted on the aromatic ring of CBD.

Our task in the research group was to investigate if the newly synthesized molecules (CBD1, CBD2, CBD3) can protect cardiomyocytes from oxidative stress on H9c2 rat heart cells.

An MTT assay was performed to determine the viability of cardiomyocytes treated with the test compounds. Trypan blue exclusion and lactate dehydrogenase (LDH) release assays were carried out to study the effect of the new derivatives in cells exposed to H_2O_2 or hypoxia/reoxygenation (H/R) compared to CBD. The direct antioxidant activity was evaluated by a total antioxidant capacity (TAC) assay. Finally, to investigate antioxidant protein levels including heme-oxygenase 1 (HO-1), superoxide dismutase (SOD), catalase western blot analysis were carried out.

pIC_{50} (the negative log of IC_{50}) values were as follows: CBD1:4.113, CBD2:3.995, CBD3:4.190, and CBD: 4.671. This means the new molecules are slightly less toxic than the parent molecule. Most of the compounds protected the cells from H/R damage, and also from the H_2O_2, especially CBD2 in the concentration of 3 and 10 µM. Among the molecules the CBD had the most potent direct antioxidant activity. The levels of antioxidant proteins were increased variously after the pretreatment of the cells with the newly synthesized CBD derivatives and CBD itself. Taken together, our new compounds are able to decrease cytotoxicity during different conditions of oxidative stress, and H/R. The new CBD analogs have comparable or even better effects than CBD on H9c2 cells.

Since the new analogues possess direct antioxidant activity, we were curious to study the effect of different substitution on antioxidant activity and cell survival. Thus, we continue the research with six new CBD derivatives containing fluor, that were synthesized recently. Some of the compounds apparently have comparable antioxidant activity indicated by FRAP and ORAC assay. Based on the in vitro results the most potent molecules will be studied in ex vivo experiments with isolated rat heart.

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Leveraging Bioinformatics Tools for the Discovery of Novel Anti-Malarials

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Abstract

Chemists throughout the world have already created a vast number of synthetic substances. Databases provide access to a large number of these compounds' 2D and 3D structures. The RCSB Protein Data Bank and other databases are collecting a growing number of publicly available protein structures as X-Ray crystallography, NMR, and in-silico modelling techniques progress.

Chemists can create effector small molecule ligands against a variety of macromolecular structures as prospective therapeutic targets. Instead of constantly synthesizing new molecules, we may use small molecular structure databases of previously synthesized molecules to screen them against protein targets utilizing in-silico virtual screening methods. This virtual developing and screening procedure on a computer screen saves time, effort, and money while also expediting the drug development process.

*pf*DHFR and *pf*ENR were chosen as targets for discovering novel antimalarial drugs. Two distinct specialized small molecule databases including di and tripeptide sequences and diaryl amides were created internally for screening against these targets. The lead compounds found by computational methods were produced, evaluated, and modified to enhance and optimize their properties. An analysis of two computational design and screening methods is provided, along with the primary compounds identified by each.

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Antimalarial Delivery with Ferritin-Based Protein Cage: A Step Towards Developing Smart Therapeutics Against Malaria

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Abstract

Over the past two decades, the utilization of protein cages has witnessed exponential growth, driven by their extensive applications in biotechnology and therapeutics. In the context of the recent Covid-19 pandemic, protein cage-based scaffolds played a pivotal role in vaccine development. Beyond vaccines, these protein cages have proven valuable in diverse drug delivery applications, thanks to their distinctive architecture and structural stability. Among the various types of protein cages, ferritin-based cages have taken the lead in drug delivery applications. This is primarily attributed to their ease of production, exceptional thermal stability, and non-toxic nature. While ferritin-based cages are commonly employed in anti-cancer drug delivery and contrast agent delivery, their efficacy in malarial drug delivery had not been explored until this study. In this investigation, several anti-malarial drugs were encapsulated within horse spleen ferritin, and the binding and loading processes were validated through both experimental and computational techniques. The data unequivocally demonstrates the facile incorporation of anti-malarial drugs into ferritin without disrupting its three-dimensional structure. Computational docking and molecular dynamic simulations were employed to pinpoint the precise location of the drug binding site within ferritin. Subsequent efficacy testing on Plasmodium revealed that the developed nanoconjugate, comprising the drug-ferritin conjugate, exhibited significant effectiveness in eradicating the parasite. In conclusion, the findings strongly indicate that ferritin-based carrier systems hold tremendous promise for the future of antimalarial drug delivery, offering high selectivity and limited side effects. In my presentation I will showcase our recent findings in protein cage based drug delivery.

Keywords: Protein cage, Ferritin, Antimalarial drug delivery, fluorescence spectroscopy, thermal stability, docking and MD simulation, *in-vitro* anti plasmodial activity, Anti-malarial therapeutics

Illuminating The Destabilization Mechanism of Small-Molecule Inhibitors Against α–Syn Oligomers in Parkinson's Disease Using Molecular Dynamics Simulations

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Abstract

The intracellular neuronal aggregates comprising α–Synuclein (α–Syn) protein known as Lewy bodies and Lewy neurites are the key hallmarks of Parkinson's disease (PD) [[i]]. The destabilization of pre-existing disease-relevant α–Syn fibrils is considered a potential therapeutic strategy against PD (Fig. 1) [[ii]]. Ellagic acid (EA), a natural polyphenolic compound, is experimentally proven as a potential candidate that reverses the α–Syn fibrillization [[iii]]. Hydroxytyrosol (HT), 3,4-dihydroxyphenylethanol, is a naturally occurring polyphenol that lessens the severity of PD by reducing α–Syn aggregation and destabilizing the pre-formed toxic α–Syn oligomers [[iv]]. Continuing with our investigations on elucidating the inhibitory mechanism of various inhibitors against Aβ aggregation and protofibril destabilization [[v]], molecular dynamics (MD) simulations have been performed in this work to illuminate the destabilization mechanism of EA and HT on α–Syn oligomers [[vi]]. EA interacted primarily with the non-amyloid-β component (NAC) of α–Syn oligomer, disrupting its β-sheet content with a concomitant increase in the coil content. The E46–K80 salt bridge, critical for the stability of Greek-key-like α–Syn fibril, was disrupted by EA. HT binds favorably to α–Syn trimer ($\Delta G_{binding}$= –23.25 ± 7.86 kcal/mol) and a notable reduction in the interchain binding affinity of α–Syn trimer on the addition of HT depicts its potential to disrupt α–Syn oligomers. The computational studies investigating the effect of small molecules on the destabilization of oligomers of varying sizes are worthy for gaining insights into the discovery of new inhibitors of α–Syn aggregation and protofibril destabilization in PD.

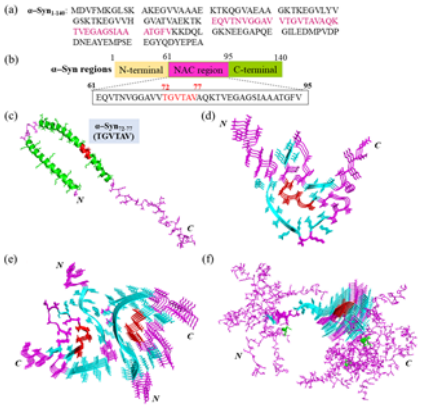

Fig. 1: Amino acid sequence of α–Syn with NAC region (residues 61–95) in pink (panel a). The different regions of α–Syn are shown in panel b. The α–Syn monomer (PDB ID: 1XQ8), α–Syn trimer (residues 37–99) obtained from the cryo-EM derived α–Syn hexamer structure (PDB ID: 6A6B), α–Syn fibril structure (PDB ID: 6CU7), and solid-state NMR structure of a pathogenic fibril of full-length α–Syn (PDB ID: 2N0A) are shown in panels c, d, e, and f, respectively.

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ZINC1250228067: A Promising Therapeutic for Permanent Vision Loss

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Abstract

Glaucoma, an ocular disorder that is widely prevalent, poses a significant menace to global ocular well-being, manifesting as a collection of pathologies that affect the optic nerve and result in irreversible visual impairment [1]. This occurrence serves as a noteworthy catalyst for visual impairment at a global level, impacting a staggering population of 76 million individuals, with a notable focus on Asia and Africa [2]. About 10% of all occurrences of irreversible visual impairment globally can be ascribed to the presence of glaucoma. The current targets for therapeutic management of glaucoma emphasize the potential intervention pathways offered by PDE, Rho kinase, and GSK3β [3].

Glycogen synthase kinase-3β (GSK3β) is involved in multiple pathways, which makes it difficult to target it specifically for a disease. However, GSK3- beta plays a crucial role at the time of glaucoma. This kinase provides neuroprotective effects on retinal ganglionic cells and photoreceptors; which underscores its significance in glaucoma treatment. Several small inhibitors have been employed to target GSK3, but they have side effects that have prevented FDA approval of those inhibitors for glaucoma treatment. Diarrhoea has appeared to be a consistent side effect of these inhibitors, with nausea, fatigue and headaches also being reported [4]. This emphasizes the need for identifying a better inhibitor with enhanced binding affinity at the target site. Our study identified ZINC1250228067 (SellesCheck_30666_1) as a promising GSK3β inhibitor, displaying potent behaviour, a favourable docking score, and high binding affinity, thereby paving the way for potential drug for glaucoma treatment.

In conclusion, we conducted an extensive in silico screening and molecular dynamics simulations investigation to discover potential inhibitors against GSK3-β. It is important to note that ZINC1250228067 emerged as an exceedingly promising candidate, as demonstrated by its impressive docking scores of -8.85 and an MMGBSA binding score of -115.75 kcal/mol. Particularly noteworthy is the fact that its MMGBSA binding energies were even lower in comparison to those of the reference compound, ZINC64532059, which displayed a docking score of -8.12 kcal/mol and an MMGBSA binding energy of -107.85 kcal/mol. These findings strongly corroborate the potential efficacy of the recently discovered inhibitor for GSK3-Beta, hence initiating opportunities for further investigation. The main goal of our study is to contribute to the discovery of new inhibitors for GSK3-beta that can be used for the treatment of glaucoma, with the potential to advance more effective therapeutic interventions.

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SARS-CoV-2: Efforts of drug design and drug discovery

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Abstract

SARS-CoV-2 is a novel coronavirus has developed quickly and caused social and economic concern. All coronaviruses, including SARS CoV-2, are large and include multiple druggable proteins. There are several important nsps that are beneficial for antiviral medications among the twenty nine proteins known to be generated by the virus: (1) PLPro and (2) 3CLPro, which are required for the formation of 16 nsps via polyprotein cleavage and functioning replication complexes. In our preliminary studies, we have virtual screened an FDA-approved library following a multi-targeting approach, which has indicated the potential of Diosmin against nsp3, nsp9, nsp12 and nsp15. Then, we designed a new in-house library of HEA compounds (>2,500) and virtual screening led to several hits against the main protease of SARS-CoV-2. The identified hits were synthesized by optimizing a novel synthetic methodology *i.e.* microwave-assisted synthesis. Later, compounds were evaluated for biological efficacy and few compounds displayed *in vitro* efficacy against SARS-CoV-2 in the low micromolar range. Interestingly one of the compounds based on aniline and HEA pharmacophore displayed biological efficacy in low nanomolar range with no apparent *in vivo* cytotoxicity. The compound's *in vitro* efficacy against viral infection surpasses that of the newly licenced medicine Nirmatrelvir (PF-07321332). Thus, these compounds can act as fundamental structures to offer fresh perspectives that may improve medication development for combating COVID-19.

Keywords: SARS-CoV-2, Main protease (3CLpro), *in silico*, *in vitro*, drug discovery.

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Preparation of Food Packaging Films Based on O-Carboxymethyl Chitosan/PVA/Hemp Fiber Filled with Neem extract: Mechanical, Antimicrobial and Biodegradation Studies

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Abstract

The development of environmentally friendly food packaging materials with enhanced functionality has gained significant attention in recent years. In this research paper, we present the eco-friendly preparation and characterization of highly degradable composite films of O-CMC (O-Carboxymethyl Chitosan) and PVA, incorporated with neem (Azadirachta indica) leaves extract and hemp fiber. The aim of this study was to investigate the tensile properties, antimicrobial activity, biodegradability, and thermal behavior of the composite films. The tensile strength and elongation at break of the films were determined using a universal testing machine. The results showed that the incorporation of hemp leaves powder improved the tensile properties of the composite films compared to the neat O-CMC and PVA films. The antimicrobial activity of the films was evaluated against a panel of microorganisms including both Gram-positive and Gram-negative bacteria as well as fungi. The composite films exhibited excellent antimicrobial activity with significant inhibition of microbial growth observed against the tested micro-organisms. Biodegradability studies were conducted by Soil burial method and the films demonstrated good biodegradability. The results of thermo-gravimetric analysis (TGA) of composite films show that they are thermally stable and might be used in food packaging.

Keywords: Active food packaging, biodegradability, mechanical analysis, neem-based composite films, thermal study.

Rapid Diagnostic Tests (RDTs) for Malaria: Why We Need New Targets Now?

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Abstract

Malaria diagnosis has been an important pillar in its control and elimination efforts. Rapid Diagnostic Tests (RDTs) are the real workhorse of detection of malaria in field settings across the globe. RDTs comprise of immobilized target-specific antibodies which forms coloured antigen-antibody complex in the presence of target antigens- histidine rich protein (HRP), lactate dehydrogenase (LDH) etc. from infected patients. Sensitivity and specificity have always been concerning issues in the use of RDTs for malaria diagnosis especially in low transmission settings. Moreover, there are now reports from Bharat regarding the deletion of Pf*hrp2*/*hrp3*- target gene for the most commonly used RDTs for *P. falciparum*. It now becomes imperative to explore new targets that can replace the HRP-based RDTs. We have recently reported two secretory proteins of *P. falciparum*- Exported protein 1 (EXP1) and Glutamate rich protein (GLURP) as potential target antigens for new age RDTs (Vashisht et al. 2022; *Translational Research*). Using protein microarray technology and ELISA, cyclic peptides from EXP1 and GLURP demonstrated potent immune-reactivity to the antibodies present in the serum of field collected *P. falciparum* infected samples. Taking this work forward, we are now in the process of developing a prototype antigen-based RDT. We have recombinantly expressed the target antigens- EXP1 and GLURP proteins and generated their polyclonal antibodies. Presently, we are quantitating the secretion of these proteins in *P. falciparum* culture in vitro as well as patients samples from diverse field sites.

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CORAL: Identification of Structural Attributes of Cannabinoid Receptor-1 Antagonists Compounds Using Correlation Contradiction Index

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Abstract

Due to its great prevalence and connection to serious health issues like diabetes, heart disease, and hypertension, obesity has drawn significant attention. According to reports, the endocannabinoid system plays a critical role in controlling energy balance, fat accumulation, and food absorption. In this publication, we describe a thorough QSAR study using the Monte Carlo optimization method built into the CORAL software for 165 CB1 receptor antagonists. The entire dataset is split into four splits, and from these splits 8 QSAR models are created using the two target functions, TF_1 (which lacks an CII) and TF_2 (which has an CII). Compared to models created with TF_1, all QSAR models built with TF_2 have more predictive potential. The model developed for split 4 using TF2 is the most advanced model because of its higher validation set $R^2_{Validation}$ = 0.9620 determination coefficient value. The CII produces statistically sound predictive models of the examined endpoint pIC_{50} and enhances the statistical performance of CORAL-based QSAR-models. Some novel compounds are designed using the recognized promoters of the increase and decrease endpoint pIC_{50} and validated using the molecular docking and dynamics.

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PE/PPE family proteins of *Mycobacterium tuberculosis* modulate host cellular pathways as molecular mimics of host proteins.

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Abstract

Mycobacterium tuberculosis (Mtb) has evolved with the host and has adopted various strategies to escape host defense mechanisms. The PE/PPE family of Mtb is exclusive to pathogenic mycobacteria. These proteins have conserved PPE residues at their N-terminus and a variable C-terminus. We have identified the presence of eukaryote-like domains or motifs in the C-terminus of dormancy-associated PPE15 and PE6 proteins of Mtb. We observed that the C-terminal regions of PPE15 and PE6 share sequence similarity with the C-terminal regions of mitochondria-targeting pro-apoptotic Bcl2 proteins and possess mitochondria-targeting signal sequences. Experiments with C-terminal region-deleted proteins confirmed their role in inducing mitochondrial stress in THP1 macrophages by depolarizing the MMP, generating mitochondrial superoxides, and depleting ATP levels. Interestingly, PPE15 was also observed to downregulate cellular ROS in host macrophages, which was correlated with the presence of a eukaryote-like SH3 (SH3e) domain and a PxxP motif in it. When the predicted SH3e-domain was deleted from the full-length protein (PPE15-/-SH3), cellular ROS and NADP/NADPH ratios returned to normal. The SH3e-domain of PPE15 was observed to interfere with ROS generation by sequestering cytosolic subunits of NOX (NADPH-Oxidase Complex) to inhibit NOX assembly at the cell membrane. These observations suggest that PPE15 and PE6 are molecular mimics of pro-apoptotic host proteins that mediate host macrophage apoptosis, and PPE15 is also a molecular mimic of the SH3e-domain, which circumvents the oxidative stress generated by the host macrophages in the late stages of infection. PPE15 and PE6 are thus identified as novel drug targets and effector proteins.

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Exploring Dengue Virus: Multi-omics Approach Using In Silico Studies

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Abstract

Dengue is a primary health concern globally and WHO has reported an 8-fold increase in dengue cases from 2000 to 2019. Dengue is caused by dengue virus belonging to Flaviviridae family, and has four serotypes. Infection with one serotype confers lifelong immunity, but subsequent infection with other serotypes causes severe dengue fever, aided by Antibody-Dependent Enhancement (ADE). Global concern for dengue stems from ineffective therapeutics availability and no accurate diagnostic method due to its diverse presentations.

Our aim was to find conserved epitopes, CpG dinucleotides and phytocompounds effective on all serotypes using in silico studies. BCPRED and BEPIPRED were used to predict B cell epitopes. In addition, we used in silico techniques to analyze 4,547 DENV genomes for novel CpG-rich regions across all serotypes. AutoDockTools 1.5.6 was used to simulate molecular docking. GROMACS 2021.5 was used to simulate a protein-ligand combination.

We found six highly conserved epitopes common to all dengue virus serotypes. Our another study assisted by genome recoding, indicated conserved CpG dinucleotides in three serotypes. Comparative analysis using CAI scores showed decreased adaptive fitness of CpG-recoded DENV inside the human host. In quest of finding cure against dengue, we found phytocompounds that can help to combat dengue and effective against all serotypes. Thus, a multi-omics approach to generate and integrate novel drugs and vaccine targets spanning the serotypes of the virus was employed.

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ORAL ABSTRACTS

Recycling Of Carbon Dioxide In The Atmosphere To Control Global Warming And Energy Crisis

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Abstract

World is facing two major problems of global warming and scarcity of energy resources. The conventional fuels such as petrol, diesel, coal, kerosene, natural gas, etc. generate carbon dioxide on burning, resulting in global warming, which causes a number of catastrophs such as melting of glaciers, rising of sea level, chilled winter, extremely hot summer, etc. This is all due to increasing amount of carbon dioxide in the atmosphere. On the other hand, increasing demand of energy sources has posed a threat of shortage of natural fuels. Both these problems can be solved by reducing carbon dioxide to useful synthetic (alternative) fuels like formic, formaldehyde, methanol and methane. These fuels on burning in fuel cells produce electricity and carbon dioxide back. The electricity so generated can be utilized for any work i.e. mechanical, sound, heat, light, etc. Therefore, it can be considered a short term loan of carbon dioxide from atmosphere. Photoreduction of carbon dioxide in presence of semiconducting materials (photocatalyst), which can serve this purpose.

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Use of Nanostructure Modified Graphitie Carbon Nitride (g-C3Na) as an efficient Photocatalyst in Wastewater Treatment

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Abstract

Graphitic Carbon Nitride (g-C,N,) has attracted the attention of scientific community all over the world in recent years due to éits exciting unusual properties and promising applications as an efficient photocatalyst for remediation of pollutants. Many modifications have been made to enhance its photocatalytic activity. The band gap of Graphitic Carbon Nitride (8-CaN,) is 2.7 ev, (Ohich is suitable for visible light driven photocatalysis ut as a pure g-CaN,, the fast electron-hole recombination and lens surface area limits its use as an effective photocatalyst. The nanocomposites of g-C3N, have shown to put a check on the recombination of photogenerated charge carriers (clectron-hole) which culminated in the increase in the photocatalytic activity of graphitic carbon nitride in the degradation of water/effluents from dye industrics.

Keywords: Photocatalysis, Graphitic Carbon Nitride, Pollutant degradation, Semiconductor with Visible light.

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Psychochemistry: The Role of Good and Bad Hormones

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Abstract

Psychochemistry is the study of the chemical processes that underlie psychological phenomena. It is an interdisciplinary field that combines elements of psychology, neuroscience, and biochemistry to explore the biochemical basis of behavior. It is important to learn the implications of psychochemistry for understanding mental health and illness. The basics of Neuro-Linguistic Programming (NLP) to understand the role of psychochemistry will be discussed. NLP is a form of psychotherapy that focuses on the connection between language, behavior, and the mind. It is based on the idea that our thoughts, feelings, and behaviors are all connected and can be changed through the use of language. NLP is used to help people identify and change patterns of behavior that are not working for them, as well as to help them develop new skills and strategies for achieving their goals. NLP can be used to overcome anxiety, depression, trauma, illness, fear & phobia, relationship problems, etc. It is important to note that many physical and mental problems can be solved by NLP.

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Photocatalytic Degradation of Azure A Dye Using ZnO-Barium Chromate Composite in Aqueous Medium

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Abstract

Photocatalysis offers a promising and sustainable approach for the degradation of dyes in wastewater, addressing water pollution challenges and contributing to the preservation of environmental and human health. The photocatalytic degradation of cationic dye Azure A using barium chromate-zinc oxide composite as the photocatalytic material presents an innovative approach to wastewater treatment. The Effect of various parameters, such as catalyst dosage, dye concentration, light intensity, pH, etc. on dye degradation was investigated. The results of the experiments showed that the reaction adheres to pseudo first
order kinetics. A tentative mechanism for the photocatalytic degradation of dye has been proposed, where superoxide anion radicals ($^{\bullet}O_2^-$) has been observed as an active oxidizing species.

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\Fluoride Ions Removal from Ground Water: Green Approach

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Abstract

Fluoride contamination in drinking water due to natural and anthropogenic activities has been recognized as one of the major problems worldwide imposing a serious threat to human health. Fluorosis is a public health problem in many parts of the world. The major source of fluoride intake is drinking water. Even though fluorosis once established is irreversible but it can be prevented through simple precaution. The permissible limit of fluoride concentration in drinking water is 1.5 mg/L according to WHO guidelines. Thus, defluoridation of water and supply of safe drinking water is the immediate solution and best preventive measure. Cost is of major consideration in developing countries like Bharat; hence, the adsorption process using bio-adsorbents was investigated which are abundant, easily available. An efficiency of different biomass for the sequestration of fluoride from water by using adsorption technique. Among several treatment technologies applied for fluoride removal, adsorption process has been explored widely and offers satisfactory results especially with mineral-based and/or surface modified adsorbents. In this review, an extensive list of various adsorbents from literature has been compiled and their adsorption capacities under various conditions (pH, initial fluoride concentration, temperature, contact time, adsorbent surface charge, etc.) for fluoride removal are presented along with highlighting and discussing the key advancement on the preparation of novel adsorbents tested so far for fluoride removal. It is evident from the literature survey that various adsorbents have shown good potential for the removal of fluoride. However, still there is a need to find out the practical utility of such developed adsorbents on a commercial scale, leading to the improvement of water pollution control.

Keywords: - Fluoride, fluorosis, Low cost Adsorbents, Contact time, pH.

Phytocatalytic Degradation of Malachite Green using Titanium Dioxide-Nickel Vanadate Composite

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Abstract

In this work, the photocatalytic degradation of Malachite Green by heterogeneous photocatalytic process using Titanium Dioxide-Nickel Vanadate Composite as semiconductor has been investigated. The effect of various parameters such as catalyst loading, pH, light intensity and concentration of the dye has been studied on the rate of reaction. Kinetic studies reveal that the photocatalytic process follows pseudo-first order kinetics. A tentative mechanism for the photocatalytic degradation of Malachite Green was proposed.

Keywords: Malachite Green dye, Nickel Vanadium Oxide, and Titanium Dioxide Composites, Photocatalytic Degradation

Improved Photovoltaic Performance of Dye-Sensitized Solar Cell (DSSC) Using Copper and Nitrogen Co-Doped Titania as Electrode

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Abstract

In recent years renewable solar energy is considered to be an environment friendly source because it directly converts solar energy into electrical power leaving no effect. Among all the solar cells DSSC has attracted much attention due to low-cost production, easy fabrication process and relatively high conversion efficiencies. Copper and nitrogen (source Liq. NH 3) co-doped and pure TiO 2 were prepared through a sol-gel process. Both pure and doped semiconductors were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FTIR) techniques, transmission electron microscopy (TEM) and diffuse reflectance spectra (DRS). The photoanode was prepared by coating of Cu–N–TiO 2 on the layer FTO conductive glasses using Rhodamine B dye as sensitizer. Electrolyte I – /I 3 – redox couple and carbon (graphite) were used as counter electrode. The co-doped electrode sensitized with Rhodamine B dye showed the open circuit voltage (Voc) = 480.0 mV, short circuit current (isc) = 0.0543 mA, Vpp = 186.7 mV and ipp = 0.0157 mA with FF = 0.11 and power conversion efficiency (η) 0.0040% under 60 mWcm –2 light intensity.

Keywords: Dye sensitized solar cell, titanium dioxide, co-doped, copper sulphate, nitrogen, FTO glasses and sensitizer.

Oxidative Stress Induced Albumin Modifications a Prognostic Biomarker in the Patients with Nonalcoholic Fatty Liver Disease (NAFLD)

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Abstract

Backgrounds: In the absence of any symptomatic clinical features, liver biopsy remains the gold standard to assess disease progression in NAFLD patients. Oxidative stress is postulated to play an important role in liver disease progression. Albumin is the most abundant plasma protein with antioxidant activity. Redox modification at free –SH group of albumin modulates its physiological function, as well as serves as a biomarker for oxidative stress.

Aim: To develop a noninvasive diagnostic plasma marker for NAFLD progression.

M**ethods:** We analyzed purified plasma albumin from 26 biopsy-proven NAFLD patients [17 with benign fatty liver and 9 with NASH] and 15 healthy controls. The analysis involved using a LC-ESI-MS system to obtain multicharged spectrum of HSA, which was deconvoluted to identify isoforms. Percent relative quantitation of albumin's isoforms were calculated and compared between groups.

Results: Three most prominent isoforms of albumin were observed in the deconvoluted spectrum with molecular masses of 66,438±2.8, 66,559±4.8 and 66,603±6Da. Unmodified albumin (m/z 66,438±2.8) was the predominant peak in healthy subjects in perfect agreement with calculated theoretical mass (66,438Da,542aa). In contrast, the percent relative abundance of modified form with addition of +119Da (cysteinylation, m/z 66,556±1.8) of albumin was significantly higher in NAFLD patients [100%v/s52±8 ($p>0.05$)]. Further, unmodified albumin was also higher in fatty liver when compared with NASH patients ($p>0.05$).

Conclusion: Our results showed that sustained oxidative stress is reflected by high levels of cysteinylated albumin in NAFLD patients and might be a useful prognostic marker to assess the degree of oxidative damage, inflammation and severity of the disease.

Dedicated to our beloved Late Prof. Ashok K. Prasad

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Diastereoselective Synthesis of Sugar infused Pyrano[3,2-*c*]Quinolones

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Abstract

Pyranoquinolones and conjugated pyrano[3,2-*c*]quinolone motifs are commonly encountered in a wide range of pharmacological drugs, synthetic materials, and bioactive natural compounds.[1,2] Pyrano[3,2-*c*]quinolones are notably acknowledged for their anticancer properties, as well as their antimalarial and antibacterial activities.[3,4,5] We intend to synthesize diastereoselective pyrano[3,2-*c*]quinolone carbohydrate conjugates with enhanced bioavailability. We have developed a facile and efficient protocol for the diastereoselective synthesis for its derivatives from Perlin aldehydes and 4-hydroxyquinolones using a one-pot condensation at room temperature.

In this investigation, glucose and galactose have been employed as inexpensive starting materials to synthesize two sets of pyrano[3,2-*c*]quinolone based carbohydrate conjugates in good to excellent yields. The reaction exhibited remarkable diastereoselectivity, resulting in a single diastereomeric product with a diastereomeric excess (*dr*) 97:3 for glucose, while a diastereomeric mixture with a diastereomeric excess (*dr*) 67:33 was obtained for galactose. Additionally, the scalability of the protocol has successfully been demonstrated by synthesizing one of the derivatives on a gram scale, highlighting its potential for large-scale production.

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Synthesis, Characterization and Biological Screening of Novel 1, 2, 4 Triazole Derivatives.

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Abstract

In the present study a series of novel triazole derivative were synthesized and evaluated for antimicrobial and anticonvulsant activity. The entire synthesized compound NJ-01, NJ-02, NJ-03, NJ-04, NJ-05, NJ-06, NJ-07, NJ-08, NJ-09, NJ-10, NJ-11 and NJ-12 were characterize by IR, 1 HNMR, and MASS spectral. Newly synthesized compounds were screened for their antibacterial (Staphylococus aureus, Bacillus sublilis (Gram postive bacteria) *Escherichia coli*, *Psedomonas aeruginosa* (Gram negative bacteria) and antifungal (Candida albicans) activity. The anticonvulsant activity determined by maximal ectro shock (MES) induced method. The result revealed that,compound NJ-01, NJ-05 and NJ-09 showed maximum growth inhibition activity against bacteria and fungi, and show seizure protection and showing quick onset of action.

Keywords: Triazole Derivatives ,Benzoic Acid, Anticonvulsant activity ,Antimicribial Activity, *Pseudomonas aurugiosa* and *Candida albicans*.

Identification of Novel Compounds from Olea Europaea: Molecular Docking and Molecular Dynamics Study

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Abstract

Cancer continues to pose a substantial worldwide health obstacle, with estimates suggesting that there will be 19.3 million new cases by 2025, primarily as a result of changes in lifestyle and longer life spans. An unexplored molecular mechanism that may contribute to the growth of cancer is the enzyme Human tRNA-dihydrouridine synthase 2 (hDus2). hDus2 has a crucial function in modifying tRNA by converting uridine residues into dihydrouridine, providing flexibility and increasing the efficiency of protein synthesis. The presence of increased levels of dihydrouridine in tRNA has been associated with the advancement of cancer, indicating that hDus2 could be a promising target for therapy. The focus of our work is to explore the suppression of hDus2 activity as a novel method for cancer treatment. We employed in-silico methods to analyse all compounds present in OliveNet Database for their affinity against hDus2. Using the Glide module, we conducted structure based virtual screening on the three-dimensional structure of hDus2. The most prominent compound was chosen for Molecular Dynamic Simulations (MDS) investigations. The binding of the lead compound to hDus2 was validated by calculating various metrics, including RMSD (Root Mean Square Deviation), RMSF (Root Mean Square Fluctuation), Principal Component Analysis (PCA), and binding free energy. The results emphasised Jaspolyoside, a recognised antioxidant, as a highly potential hDus2 inhibitor due to its significant binding affinity. Jaspolyoside, alone or in combination, can be used for the development of potent and specific
inhibitors of hDus2 for cancer therapy.

Keywords: Anti-cancer compounds, hDus2, Molecular Docking, Molecular Simulation,

Harmony in the Heat: Unraveling the Symphony of Heat Shock Protein 70 in Bharat Malarial vector- A Molecular Ballet Shaping Mosquito Development and Influencing *Plasmodium berghei* Transmission

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Abstract

This study explores the multifaceted role of Heat Shock Protein 70 (HSP70) in *Anopheles culicifacies*, a significant vector in the transmission of malaria. Through a comprehensive bioinformatic and biochemical analysis, we aim to elucidate the involvement of HSP70 in various stages of mosquito development and its impact on the life cycle of *Plasmodium berghei* within the mosquito host. The study employs inhibitors targeting HSP70 at different developmental stages of the mosquito to decipher its regulatory functions. Our research involves the integration of bioinformatics tools to predict and analyze the structural and functional aspects of HSP70 in *Anopheles culicifacies*. The biochemical characterization includes expression patterns throughout mosquito development, activity of HSP 70 functional protein and interaction with its co-chaperone HSP40 . Moreover, we investigate the influence of HSP70 inhibition using certain inhibitors to discern its role in modulating critical processes during mosquito maturation. A significant aspect of this study is the evaluation of the impact of HSP70 inhibition on *Plasmodium berghei* development within the mosquito. By employing a multidisciplinary approach, we seek to unravel the intricate interplay between HSP70 and the malaria parasite, shedding light on potential vulnerabilities that can be exploited for vector control strategies. This research not only contributes to our understanding of the molecular mechanisms governing mosquito development but also provides insights into novel strategies for disrupting the transmission of malaria. Ultimately, our findings may pave the way for the development of targeted interventions aimed at disrupting the intricate relationship between Anopheles , HSP70, and *Plasmodium berghei*, thereby advancing efforts to combat malaria on multiple fronts.

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D7L3 interaction with HSP70: A Potential Facilitator in Mosquito Blood Feeding

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Abstract

The salivary gland of the hematophagous Nematocera expresses abundant D7 proteins which function to impair the host inflammatory response by binding to biogenic amines and eicosanoid compounds produced during blood feeding. Members of D7 protein family are distantly related to insect Odorant-Binding Proteins (OBP) which is divided into short forms and long forms, containing one or two OBP-like domains, respectively. Crystal structure of several short and long form of D7 in *Anopheles darlingi* (PDB ID: 7TX8), *Anopheles stephensi* (PDB ID: 3NHT and 3NGV), *Anopheles gambiae* (PDB ID: 2QEV), *Aedes aegypti* (PDB ID: 7TVC, 3DYE, 3DZT) have been deciphered wherein, the proteins were expressed as inclusion bodies in various eukaryotic and prokaryotic heterologous hosts. Intrigued by this, we looked for the possible interaction of D7 proteins with chaperon proteins in the Bharatn malarial vector; *Anopheles culicifacies*. Interaction studies involving one of the long forms of D7 protein (D7L3) revealed highly specific interaction with HSP70 via Dot Blot and ELISA. This was further substantiated by MicroScale Thermophoresis wherein, the D7L3 binds to HSP70 with binding affinity (Kd) ≈3.4 µM. The interaction of the D7L3 and HSP70 is to be further validated by gel permeation chromatography and crystallization of the protein complex. Prima facie we hypothesize that HSP70 alone or in complex with other molecular chaperons promotes the stability of D7L3 in the salivary gland of blood feeding arthropods, thus facilitating blood meal acquisition.

***Keywords*:** D7L3, Heat Shock Protein 70, *Anopheles culicifacies,* Binding affinity

A Review on Reproductive Disease Management with Herbal Drugs: Strategies and Results

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Abstract

Reproductive disease is a disease of male and female reproductive system. This system is made up of organs and glands that make hormones, like the pituitary gland in the brain. Reproductive organs or gonads, such as the ovaries in females and the testicles in males, maintain the health of their respective systems because they also serve as glands and produce hormones. The reproductive system is susceptible to various diseases which may develop during multiple phases of life. Female disorders include, early or delayed puberty, endometriosis, cancer, infertility, polycystic ovarian syndrome, problems during pregnancy, uterine fibroids and menstrual irregularities. Male disorders include, erectile dysfunction, cancer and low sperm count. Herbal are regarded as one of the most important branches of traditional system of medicine, it plays a significant role in health care systems. Herbal drugs are actually regarded as a crucial area of pharmacy and medicine, and in addition, the plants used in herbal drugs are important sources for the pharmaceutical industries research into pharmacologically active drugs. Additionally, interest in using this kind of medicine is steadily rising among the general public worldwide, due to its accessibility, affordability, and range of health benefits, herbal drugs was used by about 80% of people in developing countries. The therapeutic efficacy of various herbal drugs in the treatment of different types of reproductive diseases has been studied. In this review we focus on herbal drugs which are used for the management of male and female's reproductive diseases.

***Keywords*:** reproductive dysfunctions, PCOS, prostate cancer, endometrial cancer, menstrual irregularities.

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Marine Bacterial Formulations Exhibit Specific Larvicidal and Ovicidal Activity Against Bharat Malaria Vectors.

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Abstract

With insecticide resistance on the rise, lack of novel bioactive compounds against the malaria vector, *Anopheles*, remains a serious problem. Chemical insecticides also face issues including effect on non-target species. Natural products, especially marine extracts, remain less explored for their potential bioactivity against various pathogens. Bharat, surrounded by three different marine bodies present a treasure trove for novel bioactive compounds. In this study, we have discovered a number of promising marine bacterial extracts collected and tested in collaboration with CSIR-National Institute of Oceanography (NIO), Goa, and assessed their larvicidal activity against *Anopheles stephensi* and *Anopheles culicifacies*. One of the extracts (NIO 706) displayed 100% mortality against a field strain *A. subpictus* at 125 ppm, indicating good translational potential. Moreover, one of the marine bacterial extracts (NIO 740) displayed significant ovicidal activity against *A. stephensi* and *A. culicifacies* that reduced the number of eggs hatched to almost 4%-7%. Mass spectrometry analysis of larvae lysates treated with a specific marine bacterial extract (NIO 97) belonging to *Bacillus* spp., identified a potential target. Bioinformatics analysis revealed this protein as the Hexamerin-2 beta analogue in Aedes. Collectively, these results show the importance of marine natural extracts as effective inhibitors against the development of larvae to adult stage mosquitoes.

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Pattern of Hepatic Dysfunction in Scrub Typhus Patients in Udaipur

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Abstract

Scub typhus is a zoonotic illness caused by Orientia tsutsugamushi, a gram negative proteobacterium. It is transmitted by the bite of larval stage of trombiculid mites also known as chiggers. Mostly located in the foothills of Himalayas previously but now much prevalent in tropical and south Rajasthan. Several studies have describe the clinic pathological profiles of Scrub Typhus in this subgroup of population. We hereby focus on the hepatic dysfunction including fulminant liver failure in our group patients. It was observed that majority of these patients present with subclinical liver dysfunction with/without jaundice. Thus we focussed primarily on representation of retrospective analysis of various parameters of hepatic dysfunction in almost 75 patients admitting in our hospital with serologically proven scrub typhus infection. This is an initial analysis of the study.

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Green Synthesized Insulin-Infused Bimetallic Nano-subclusters as Multifunctional Agents for ROS Scavenging, Antibacterial Resilience, and Accelerated Diabetic Wound Healing

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Abstract

This is the first report on the synthesis and wound healing application of green synthesized insulin-infused bimetallic (copper-silver) nano-subclusters (ICu-AgNSCs) with high stability, aqueous solubility, biocompatibility, and target specificity. HRTEM and SAED data confirm octahedral particles (with diameter of 9.6 ± 2.2 nm) composed of discrete copper clusters on the periphery and silver core that are further infused with insulin (0.5 ± 0.2 nm) corona, as confirmed by the characteristics Cu-OH and Ag-O stretching bonds and alteration in insulin amide bonds. The ICu-AgNSCs had high insulin loading efficiency (93.90 ± 1.05 %) and drug release rate (92.69 ± 0.90 % within 40 h), allowing it to be ideal for sustained release applications. Wound healing in diabetic conditions gets delayed due to the prolonged proinflammatory phase and microbial infestation, which may lead to clinical amputation. Therefore, advanced therapeutics that promote cell growth by reducing inflammation and microbial growth are required. ICu-AgNSCs may satisfy all these criteria. Insulin and quercetin have ROS scavenging and anti-inflammatory properties. Insulin and copper have cellular growth-promoting activity; additionally, silver has antimicrobial properties. Together, ICu-AgNSCs, have been shown to accelerate diabetic wound healing *in vitro,* making them an ideal choice for pre-clinical and clinical applications.

Keywords*:* Bimetallic nano-subclusters; Wound healing; Antioxidant activity; Antibacterial agent; Green synthesis; Protein-protected nanoclusters.

Air Pollution Measurement of Lake City Udaipur During Diwali Season.

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Abstract

Short-term investigations of atmospheric pollutants (PM_{10}, $PM_{2.5}$, SO_2, NO_2, O_3, and CO) were performed during the Diwali festival over Lake City Udaipur. We studied the data from January 2023 to December 2023, for 1 Year. In this study we have covered the air pollution parameters in Udaipur city during time of Jan 2023 to Dec 2023 including Diwali season. We observed the changes in the air pollution and its relativity with the Diwali season. Udaipur, the lake city of Rajasthan is a well-arranged city of Bharat. We chose to observe parameters of Udaipur because of various number of lakes and it is less pollute then other metro cities. The globe is now experiencing extraordinary problems with regard to the deterioration of air quality because of a significant increase in anthropogenic emissions linked to fast industrialization, motorization, urbanization, and inadequate knowledge of air health. Because of the health risks and high concentrations of pollutants, the quality of the air in megacities and other large population centers is a major problem. Bharat's high levels of air pollution emissions are also an inevitable consequence of the country's fast economic expansion and growing population. The scientific community has recently been more aware of short-term episodes of air quality degradation, and they are becoming a hot issue for discussion at all levels. Around the world, fireworks are widely utilized to commemorate a variety of holidays, including Bharat's Diwali Festival.

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Phytochemicals as a Potential Strategy to Treat Breast Cancer

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Abstract

Breast cancer is recognized as the second most commonly diagnosed cancer on a global scale, and it has emerged as an increasingly significant issue in the field of global health in recent years. As per WCRF, the global incidence of new cancer cases in 2020 amounted to 18,094,716; new cases. Among these cases, breast cancer accounted for 2,261,419 (12.5%) instances, representing approximately 12.5% of the total cases. The existing available therapeutic methods of breast cancer treatment are majorly surgical tumor removal of the tumor, stem cell transplantation, radiation therapy, gene therapy, targeted therapy, palliative care, hormonal therapy, and using various chemotherapeutic agents like paclitaxel, cyclophosphamide, doxorubicin, etc. These therapeutic methods have multiple limitations along with various side effects like loss of hair, fatigue, vomiting, pain, nausea, gastrointestinal problems, and alterations in body weight. The major limitations of the classical treatment methods include drug resistance development, recurrence of the tumor, failure to destroy breast cancer stem cells (bCSCs), metastasis of the tumor to other organs, etc. These limitations decrease the efficiency of current therapeutic strategies and demand the search for more efficient and harmless methods of breast carcinoma treatment. Phytochemicals which are bioactive natural substances found in both non-dietary and non-dietary plants, are emerging as potential agents for combating cancer and inhibiting metastasis and as safer alternatives against breast cancer. This work herein presents the *in-silico* screening of phytochemicals against breast cancer metabolic enzyme lactate dehydrogenase A (LDHA) as a potential strategy against breast cancer.

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Plant Extracts as Green Corrosion Inhibitors for Corrosion of Iron and Steel

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Abstract

This research work is on the experiment to know the corrosion inhibition effects of aerial parts that are leaves of *Momordica dioica* on Iron (Fe) through the medium of sulphuric acid. This plant is of the Cucurbitaceae family and commonly known as the Spine Gourd in different regions of South Asia. The methods and materials of the experiments have been demonstrated in this research paper and the observation presentation indicates to the affectivity of the leaf extract of *Momordica dioica* as the corrosion inhibitory natural product.

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A Comprehensive Review on Alzheimer's Disease

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Abstract

Alzheimer's disease is a prevalent and dangerous form of dementia, with its incidence increasing due to sedentary lifestyles and processed foods. While no complete cure exists, global efforts aim to mitigate its effects. Current treatments target symptoms and specific biomarkers. Several hypotheses explain its pathology, including the Cholinergic, Amyloid-β, Tau, Mitochondrial cascade, and oxidative stress hypotheses as the major ones. Recent research has produced promising therapeutics and repurposed FDA-approved drugs, aligning with these hypotheses. Efforts are focused not just on developing therapeutic directly, but also on improving drug delivery methods, legal consent by subjects for trials, early detection techniques for investigating biomarkers, and leveraging AI and machine learning for target identification. With emerging interventions, we have also included unconventional approaches such as balancing the right levels of Gut microbiota, supplementing brain function mediators, and using natural products, etc.; they are showing positive effects in many studies. Due to Alzheimer's complexity, the way to complete a cure poses challenges, but multidimensional research offers promising prospects for a cure shortly. The future looks optimistic, aiming for a complete cure with breakthroughs like those discussed in this review.

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AI-driven Strategies for Therapeutic Advancements in Amyloidal Disorders: From Drug Discovery to Personalized Medicine and Clinical Trial Optimization

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Abstract

AI-driven strategies for therapeutic development in amyloidal disorders encompass diverse methods. In the realm of drug discovery, the use of virtual screening and generative models accelerates the identification of potential compounds that target amyloid aggregation [1]. Cutting-edge AI models, such as AlphaFold, play a pivotal role in predicting protein structures, a crucial aspect of drug design [2] . Machine learning is applied to analyze extensive datasets, identifying biomarkers for early disease detection and monitoring. Personalized medicine utilizes AI to customize treatments based on individual patient data. Text mining and knowledge graphs are employed to repurpose drugs by extracting pertinent information from scientific literature. In the context of clinical trials, AI optimizes patient recruitment and predicts treatment responses, enhancing overall trial efficiency. Apart from this AI offers biomarker discovery, precision medicine etc.

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Metal-Free Construction of Aminated Isoquinoline Frameworks from 2-(2-oxo-2-arylethyl) Benzonitrile in an Aqueous Medium

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Abstract

Herein, we report a metal/additive-free protocol for the activation of nitrile towards the nucleophilic addition and subsequent annulation under an aqueous medium for the first time. The protocol divulges an efficient and atom economical route for the construction of diversified aminated isoquinolines. Differently substituted primary as well as secondary amines underwent the reaction in a highly regioselective manner. The reaction is operationally simple, shows high functional group tolerance, easier modification of well-known drugs, and successfully extended to gram-scale synthesis.

Keywords: Metal-free, Aminoisoquinoline, Annulation, Green solvent

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Biomimicry: A Path to Sustainable Innovation

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Abstract

Biomimicry, the practice of emulating nature's designs and processes to solve human challenges, has emerged as a promising avenue for sustainable innovation. This abstract explores the role of biomimicry in fostering environmentally friendly solutions and sustainable technologies. It emphasizes the potential of biomimicry to inspire creative problem-solving, reduce environmental impact, and contribute to the development of sustainable practices.

Biomimicry in drug design is an innovative approach that draws inspiration from nature's biological systems. By studying the molecular structures, processes, and functions found in living organisms, researchers aim to create pharmaceuticals that mimic or adapt natural mechanisms for therapeutic purposes. This approach leverages the efficiency and specificity evolved in biological systems, potentially leading to the development of safer and more effective drugs.

For a sustainable design, it is necessary to consider water efficiency, zero waste, thermal environment, and energy supply. Biomimicry harnesses and replicates the principles found in nature to create a built environment that benefits people and other living creatures and safeguards biodiversity. Through a comprehensive review of relevant literature and case studies, we highlight the importance of integrating biomimicry into the realm of sustainable innovation.

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Stability of L-Ascorbic Acid in aqueous solutions of salts: An Electronic Spectroscopic Study

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Abstract

Ascorbic acid, also referred to as Vitamin C, is a water-soluble antioxidant that is crucial for the growth, development, and repair of tissues. The stability of this molecule can be influenced by various circumstances, such as pH, temperature, and other variables.

Our objective is to investigate the stability of ascorbic acid when exposed to typical food additives and ions, such as Na^+, K^+, Cl^- and HCO_3^- that are naturally present in human body, via spectroscopic measurement. Physiological concentration of sodium, potassium and chloride ions has no influence on the stability.
When ascorbic acid was added to a 0.175 M HCO_3- aqueous solution, a strong peak was detected at 265.0 nm due to the presence of ascorbate anion. However, within 75 minutes, this peak disappeared completely, indicating significant decomposition. At a lower, physiological 0.035 M concentration of HCO_3^- , the peak persisted at 265.0 nm, and the rate of decomposition was slower. Our findings suggest that the elevated levels of HCO_3- in serum plasma would rapidly decompose ascorbic acid, underscoring the importance of maintaining proper physiological balance *in vivo*.

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Biochemical Constituents and Ethnomedical Potential of Parthenium hysterophorus(L.).

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Abstract

Parthenium hysterophorus is an aggressive invasive and pernicious weed that poses threat to all over the world. It shows human allergic metastasis issues, dermatitis and mutagenicity in humans and livestock. However several ancient studies have described its novel uses including several health benefits like a cure for skin inflammation, rheumatic pain, diarrhoea , tract infections, dysentery, protozoal infection, neurologic disorders, urinary tract infections, malaria and as emmenagogue and aches. It is also used as remedy for inflammation, eczema, skin rashes, herpes, rheumatic pain, cold, heart trouble and gynaecological ailments. It possesses certain allelochemicals and oils, polyphenols, alkaloids, flavonoids, terpenes, pseudoguaianolides, and histamines that shown to exhibit ethnomedicinal properties and effects. *Parthenium* can also be used as a potent herbicide, insecticide, pesticide and phytoremedial agent for metal and dye removal from industrial waste. As, *Parthenium* has various beneficial and harmful impacts. The weed also exhibits many environmental applications. Chemical constituents of *Parthenium* show extensive range of pharmacological activities suggesting its role as a chemotherapeutic agent. Its potential as a nano-medicine is being disbursed with some preliminary success to this point. Removal of contaminating heavy metals and industrial dyes, control of aquatic weeds, employment as a substrate for industrial catalyst production, additives in Cattle manure for biogas production, as a biopesticide, as green manure and compost . Although plenty of compounds were isolated from this plant, further work needs to be carried out and explore folk recipes for the benefit of improving human health.

Keywords *:* Allelochemicals, Emmenagogue, Ethnomedical, Biopesticides, Biogas

Computational Analysis Of The Ligand Binding Domain Of The Thyroid Hormone Receptor For The Rational Design Of An Efficient Protein-Based Biosensor For The Detection Of Endocrine-Disrupting Chemicals

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Abstract

Thyroid hormone-disrupting chemicals (THDCs) which are present in the environment, food and everyday consumer products, interfere with thyroid hormone signaling, possibly by interacting with thyroid hormone receptors (THRs). This alters the thyroid hormone homeostasis and affects various functions regulated by the thyroid hormone e.g. macronutrient metabolism, cardiovascular function, and normal brain development. Therefore, there is a necessity for the detection and monitoring of these pollutants in the environment. THRs belong to the nuclear receptor superfamily and have two highly conserved domains: DNA binding domain (DBD) and ligand binding domain (LBD). The LBD is responsible for ligand selectivity and could be used as a bio-recognition element in a protein-based biosensor for THDCs detection [1]. However, mutant LBD with increased affinity will act as better bio-recognition elements due to their increased sensitivity towards THDCs and capability to detect very low quantities of chemicals [2]. In our study, we used computational methods to predict the residues in thyroid hormone receptors for rational modification with an enhanced binding affinity toward a certain class of chemicals. We compiled a list of suspected THDCs and performed virtual screening against the THRs (alpha and beta) using the THR structure ensemble as a receptor in docking simulations. We analyzed the THR-THDCs interaction and selected residues that were interacting with THDCs and differentially conserved. Selected residues could be used for the rational design of LBD with an enhanced affinity towards ligands and applied towards the development of sensitive protein-based biosensors to detect THDCs. Our study will be useful in developing efficient receptors for detecting EDCs and provide insight into diseases due to mutations in the receptors.

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Evaluation of Dietary Status of Adolescent School Going Boys of Himachal Pradesh

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Abstract

The nutritional standard of the Himachali children was observed to assess the physical growth and malnutrition of adolescent school-going boys of Himachal Pradesh within the age group of 15-17 years. Boys were selected from both; government and private schools of the non- hilly regions of Mandi district of Himachal Pradesh. Height, weight, and BMI were determined. Stunting was evaluated from height-for-age Z-score, and thinness, overweight, and obesity were estimated from BMI-for-age Z-score using the WHO recommended cut- off values. Mean height varied between 167.2 to 168.7 cm. Weight varied between 52.4 to 56.1 kg with a corresponding BMI between 18.7 to 19.7 kg/m^2.The overall prevalence of stunting and wasting were 5.7 and 15.8% respectively. The coexistence of stunting and wasting was not found in any of the age groups. The overall prevalence of overweight and obesity was 5.4 and 1.7% respectively. Himachali boys appeared to be taller than most of the Indian population of boys of similar age groups. Prevalence of the different categories of overnutrition and undernutrition were also lower as compared to other Indian adolescent boys. The existence of overweight and obese individuals points towards the double burden of malnutrition.

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Elucidating the Role of Base Excision Repair Enzymes in Organellar Genome Maintenance in the Malaria Parasite

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Abstract

Malaria parasite carries two organelles, the apicoplast and the mitochondrion which contains extranuclear DNA. The genome maintenance of extranuclear DNA is required for optimal function and parasite survival under oxidative stress. *Plasmodium* parasite undergoes various stages of the parasite life cycle where replication takes place. During the replication process, exogenous or endogenous DNA damage is inescapable. DNA endures a lot of changes under the cell's chemical environment due to the presence of both internal and external stress inducers. Therefore, all cells require some form of DNA repair as a normal part of their proliferation process. Base excision repair is a conserved pathway that maintains genomic integrity by correcting the base lesions, caused by oxidative stress. This process initiated by a DNA glycosylase that recognizes and removes the damaged base, leaving an abasic site which is further processed by an apurinic/apyrimidinic endonuclease enzymes.[1] To demonstrate the role of DNA Glycosylase (Ogg1) and Apurinic/apyrimidinic (AP) endonuclease of the rodent malaria parasite in the malaria life cycle, we disrupted the genes by double-cross-over homologous recombination. The knockout parasites showed normal blood and mosquito stages development. However, inoculation of mice with Ogg1 and Ape1 knockout salivary gland sporozoites displayed a reduced capacity to initiate blood-stage infection. We found that knockout parasites undergo normal liver stage development until merozoites egress from hepatocytes. We further found that the delay in the pre-patent period was due to the inability of knockout merosomes to infect erythrocytes efficiently. We have previously shown that *Apn1* is dispensable throughout the parasite life cycle stages. There is a possibility that *Ape1* and *Apn1* compensate for the loss of each other's function. To check the cumulative effect of *Apn1/Ape1* deletion, we attempted to disrupt both genes simultaneously in *P. berghei* which failed. These results indicate that *AP endonucleases* activity is essential for parasite development in blood stages.

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A Cub and Sushi Domain Containing Protein with Esterase like Activity Confers Insecticide Resistance in Bharat Malaria Vector- *Anopheles Stephensi*

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Abstract

Chemical insecticides (organophosphates and pyrethroids) in the form of IRS (Indoor Residual Sprays) and LLITNs (lasting insecticide-treated nets) are the cornerstone for vector control, globally. However, their incessant use has resulted in widespread resistance warranting continuous monitoring and investigation of the underlying mechanism of resistance being developed by the *Anopheles* vector-prominent malaria vector. Here, we identified a previously uncharacterized- Cub and Sushi Domain containing Insecticide Resistance (CSDIR) protein and generated evidence for its role in mediating insecticide resistance in the *Anopheles stephensi.* A strong binding affinity of the CSDIR protein towards different classes of insecticide molecules-(malathion (K_D 6.43±0.013 µM) and deltamethrin (K_D 46.7µM) were confirmed using MD simulation studies and Surface Plasmon Resonance (SPR). Further, the recombinant $CSDIR^{913-1190}$ protein exhibited potent esterase-like activity (α-naphthyl acetate (α-NA)- 1.356±0.262 mM/min/mg and β-naphthyl acetate (β-NA)- 1.777±0.220 mM/min/mg). Interestingly, dsRNA-mediated gene silencing of the CSDIR transcripts caused >60% mortality in resistant *An. stephensi* upon 1 hour exposure to the deltamethrin and malathion insecticides compared to the control group. A significant reduction in the esterase-like activity was also observed against α-NA (P=0.004) and β-NA (P=0.025) in CSDIR knockdown mosquitoes compared to the control group. Using computational analysis and experimental data, our results provided significant evidence of the involvement of the CSDIR protein in mediating insecticide resistance in *Anopheles* mosquitoes. Thus, the CSDIR protein can be explored for the discovery of new insecticide molecules. These data would also be helpful in further understanding the metabolic resistance developed by the *Anopheles* vector.

Keywords: Malaria, *Anopheles stephensi*, Insecticide resistance, Esterase-like protein, Silencing

An Immunoinformatic Approach to Design a Multi-epitope Vaccine Candidate for Plasmodium falciparum Secretory Proteins.

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Abstract

Malaria has been the devastating infectious disease since ancient time, which has been a hugeburden for the healthcare sector and economy of the developing Asian and African nations. Despite the recent advancements in science and technology, Bharat contributes 1.7% of cases and 1.2% mortality. Emerging drug resistance and cerebral infection is a big concern for the growing nation. Malaria infection starts with the inoculation of the Plasmodium parasite. During the inoculation through the female Anopheles mosquito bite, the salivary gland sporozoite secretes several proteins that initiate early colonization in the hepatocytes. These secretory proteins modulate immune responses during exo-erythrocytic stage development. With this knowledge, we identified the secretory proteins with antigenic properties that are non-allergic to make a multiepitope vaccine construct. We found that these epitopes have discontinuous B cell epitopes and can generate the IgG and IgM antibodies against the Plasmodium parasite. Here we modelled a multiepitope subunit vaccine candidate against the Plasmodium secretory proteins. We identified the B cell with CTL, HTL and MHCs inducing epitopes of these proteins. We further evaluated it for immunogenicity, allergenicity, worldwide population coverage, and physiochemical characterization using different in-silico tools. Furthermore, to confirm its interaction stability, we performed molecular docking, molecular dynamics simulation, and immune simulation studies for its stable affinity with TLR2 and TLR4 receptor, which revealed a good binding affinity and immune responses.

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Investigating the Antimalarial Properties of Extracts and Compound Derived from Natural Sources

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Abstract

Malaria is potentially life-threatening parasitic disease caused by *Plasmodium* species. Natural extracts from plants, microorganisms or fungi offer diverse chemical space and often yield more hits or leads. To establish a sustainable malaria drug discovery, pipeline exploration of nature-derived antimalarials is crucial. Quinine, chloroquine, artemisinin are some of the noteworthy examples. Currently, Artemisinin combination therapies (**ACTs**) with long-acting partner drugs constitutes the radical treatment of *P. falciparum* malaria. But there are also widespread reports of the evolution of Artemisinin resistant parasites. Therefore, it is imperative to continue our exploration of nature-derived antimalarials from plants as well as from synthetic sources. This study evaluates the potency of natural extracts and isolates the active ingredients and confirm the action of the extracts by *in vitro* and *in vivo* experiments. We set out to develop a collaborative network with researchers from different institutes across Bharat and are screening large scale extracts derived from plants. After finding the hits with potent antimalarial activity, we shall perform the identification and mechanism of action elucidation of highly potent antimalarial compounds. The nature derived antimalarials have lesser chance of developing resistance by the parasite. Chemical characterization of the active fractions shall also be performed to identify the scaffolds, mode of action and target identification.

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Neddylation is Essential For Malaria Transmission in *Plasmodium berghei*

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Abstract

Neddylation is a type of posttranslational modification known to regulate a wide range of cellular processes by covalently conjugating the ubiquitin-like protein Nedd8 to target proteins at lysine residues. However, the role of neddylation in malaria parasites has not been determined. Here, for the first time, we showed that neddylation plays an essential role in malaria transmission in *Plasmodium berghei*. We found that disruption of Nedd8 did not affect blood stage propagation, gametocyte development, gamete formation, or zygote formation while abolishing the formation of ookinetes and further transmission of the parasites in mosquitoes. These phenotypic defects in Nedd8 KO parasites were complemented by reintroducing the gene that restored mosquito transmission to wild-type levels. Our data establish the role of *P. berghei* Nedd8 in malaria parasite transmission.

Keywords: *Plasmodium*; Posttranslational modification; Neddylation; Nedd8; Malaria transmission.

Implementation of Electrooxidation Technique for the Treatment of Simulated Wastewater Using MMO Anodes for Bacterial Decontamination

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Abstract

An appealing and affordable decentralized wastewater treatment system using electrochemical technology is available to eliminate the microbiological burden from contaminated water. The mixed metal oxide (MMO) anodes used in this electrooxidation (EO) technique are stablebecause these contain TiO 2 , RuO 2 , PtO 2 , and IrO 2 . This EO technique can be used in sewage pre-treatment facilities to prevent the spread of epidemics by preventing sewage water's pathogens from entering the environment. It requires a low electrolyte concentration and current. The electrochemical disinfection experiments were carried out in batch mode to evaluate the effectiveness of the EO system for inactivating eight different bacteria i.e., Salmonella enterica, Acinetobacter calcoacetius, Serratia marcescens, Listeria sp., Enterococcus faecalis, Escherichia coli, Bacillus subtilis, Staphylococcus aureus. The results showed that all eight bacteria in simulated wastewater were completely inactivated when the current density of (2.38 mA/cm 2), NaCl concentration of (1 g/300 mL), and treatment time (2 min) were maximized. Under the same optimal conditions, 100% inactivation was achieved after an 8-minute treatment of actual sewage water. To confirm that bacteria had been destroyed completely, a potassium ion leakage test and vital staining were also performed. The electrodes used in this study were shown to be durable even after 80 cycles as confirmed through FE-SEM/EDS, XRD, CV and Raman spectra. Therefore, this newly established EO system with affordable MMO electrodes may open up new possibilities for treating waterborne diseases, especially in hospital environments.

Keywords: Electro-oxidation, Simulated wastewater, Microbial decontamination, Water-based pandemic, Decentralized treatment

Palladaelectro-catalyzed C−H Activation/Arylation of Arenes using Aryl Diazonium Salts

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Abstract

The emergence of resource-economical, environmentally benign strategies is one of the primary objectives of synthetic organic chemists. This can be achieved by minimizing waste product, avoiding the use of harsh chemicals and minimizing the cost of a chemical transformation. Transition metal-electro catalyzed C−H functionalization is one of the best alternative to traditional methods. (1,2,3) This strategy is used in late-stage (4) and site-selective functionalization (5) for the assembly of complex molecules. Herein, we developed a method of palladaelectro catalyzed C−H activation/ arylation of arenes using diazonium compounds which avoids the use of stoichiometric amounts of chemical oxidants and pre-functionalized starting materials, and reduce undesired waste generation.

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Exploring Novel Pyrimidine Derivatives: Design, Synthesis, Characterization, and Pharmalogical Evaluation as Antihyperlipidemic Agents

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Abstract

Molecular docking is a computational technique utilized in the field of structural biology and drug discovery. It aims to predict the binding orientation and affinity between two or more molecules, typically a protein and a ligand (small molecule), by simulating their interaction within a defined three-dimensional space. The process involves generating multiple conformations of the ligand and exploring various binding poses within the binding site of the protein. By evaluating intermolecular interactions, such as hydrogen bonds, hydrophobic interactions, and electrostatic forces, docking algorithms estimate the binding energy and thereby predict the strength of the binding interaction. Molecular docking plays a critical role in understanding molecular recognition, deciphering protein-ligand interactions, and aiding in the discovery of potential drug candidates. The technique has wide-ranging applications, including virtual screening of compound libraries, lead optimization, and elucidating the mechanisms of molecular interactions. Through the integration of computational simulations and structural biology data, molecular docking contributes to the acceleration of drug discovery processes and the exploration of molecular interactions that underlie pyrimidine derivatives significance spars their roles in fundamental cellular processes, such as DNA and RNA synthesis, as well as their utility in drug discovery and development. These derivatives have been extensively studied for their interactions with enzymes, receptors, and other biomolecules, making them crucial components fields like medicinal chemistry and molecular biology, in drug discovery prinde derivatives have been exploited as scaffolds for designing drugs targeting a variety of diseases including cancer, viral infections inflammation, and metabolic disorders. Their versatile nature allows for structural modifications to enhance binding affinities, selectivity and pharmacokinetic properties, resulting in compounds with improved therapeutic profiles Furthermore, pyrimidine derivatives have contributed to advancements personalized medicine, as specific modifications can be tailored to individual genetic variations or disease conditions The elucidations of their molecular interactions through computational simulations and structural studies has enabled the rational designs of novel drug candidates and the optimization of existing ones various biological phenomena.

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Antimalarial Evolution of Compound Isolated from *Stachytarpheta jamaicensis* (Snakeweed) Plant

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Abstract

Since ancient times, people have utilized plants as a source of medicine to cure a variety of illnesses. In the medical systems of Bharat, Egypt, China, Greece, and Rome, there is lots of evidence supporting the use of plants as medication to cure various ailments. For example artimisnin is an anti-malarial isolated plant Artemisia annua. Pharmacognosy is the study of drugs obtained from natural sources, primarily plants, which may eventually result in the creation of novel drugs. Thus, we are inspired to investigate the chemical composition and pharmacological activity of *Stachytarpheta jamaicensis* leaf extract in order to find prospective sources for innovative anti-malarial pharmaceutical formulations. *Stachytarpheta jamaicensis* is a weedy, herbaceous plant belongs to the family Verbenaceae has significant medicinal properties. In infectious and chronic health systems, Stachytarpheta jamaicensis has been a significant herb with excellent therapeutic qualities. It exhibits a variety of bioactive phytochemical compositions, acting as an antibacterial, antioxidant, immunomodulatory, and antidiarrheal agent. With these facts, we isolated few compounds that were further subjected to in vitro and in vivo antimalarial efficacy against the Pf3D7, malaria strain. In this presentation, we will discuss the isolation, characterization (HPLC, I H-NMR, 13 C-NMR, HRMS) and biological results of all the isolated compounds.

Keyword: *Stachytarpheta jamaicensis*, anti-malarial, *P. falciparum*

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Molecular Assessment of Biodiversity of Himalayan Flora and Bioprospecting for Anticancer Agents

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Abstract

The mountainous state of Uttarakhand is endowed with a rich variety of medicinal flora belonging to diverse taxa. However, besides several well-documented medicinal plants the Himalayan region of Uttarakhand harbors a significant share of locally emerged (mostly undocumented) pharmacognosy, within the various tribes, communities, or even families. Unfortunately, in the absence of comprehensive documentation and scientific validation, this invaluable knowledge is at the verge of extinction. Furthermore, there exists threat of unauthorized commercial exploitation of these biological resources, by individuals or organizations without the permission of the source country. Therefore, we have been carrying out DNA-barcoding for the high value plants and other taxa (e.g. Lichens, endolichenic fungi, and other life-forms) of this region. Besides being helpful in species identification, these barcodes are expected to be useful in preventing biopiracy of these valuable bioresources in future.

As many of species of these life-forms are known for their anti-inflammatory potential in the traditional system of medicine; so, in view of molecular overlap between chronic inflammation and cancer progression we characterized their anti-cancer (and related) attributes. Extracts from different species of high value plants and lichens have been examined for their anti-oxidant, anti-mutagenic, anti-inflammatory, and anti-proliferative activities. The epithelial-mesenchymal transition (EMT) of tumor cells is known to induce metastasis and emergence of drug-resistance, so, we also assessed the anti-EMT potential of these species. Purification of constituent bioactive metabolites would pave way for their comprehensive activity/toxicity assessment and possible use as anticancer therapeutics, as an individual drug or under combinatorial setting.

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Novel Fluorinated Piperazine-Based Compounds: Effective Antimalarial Frameworks

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Abstract

Malaria, primarily caused by Plasmodium falciparum infection in Africa, continues to be one of the most significant infectious diseases globally.[1] While medications like artemisinin and its derivatives offer fast-acting therapeutic options, the evolution of drug resistance poses a significant global health challenge.[2] To combat malaria effectively, the drug development industry requires more potent and efficient scaffolds.[3] Fluorine exhibits several advantageous qualities in pharmaceuticals, including its small size, metabolic stability, high lipophilicity, and unique ability to extend drug half-life. Incorporating fluorine into ligands has thus become a promising strategy in medicinal chemistry.[5] Piperazine derivatives are widely studied in nitrogen heterocyclic chemistry and encompass various pharmacological agents, including those targeting the cardiovascular system, local anesthesia, analgesics, and neurotropic medications.[6] In light of these considerations, we synthesized a novel class of fluorinated-piperazine-based hydroxyethylamine (HEA) compounds. These compounds were then evaluated for their antimalarial efficacy against the Pf3D7 strain, known for its sensitivity to chloroquine (CQ). In this presentation, we will delve into the synthesis, characterization (utilizing techniques such as HPLC, IH-NMR, 13C-NMR, HRMS), and biological results of all the newly synthesized analogs.

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Effect Of Antiretroviral Therapy On Cardiac Risk Markers In People Living With HIV/AIDS

Dr. Pulin K Gupta

Abstract

Introduction: Cardiovascular diseases (CVD) are a major cause of mortality in chronic HIV infection and may be associated with classical known risk factors, direct consequence of HIV infection itself or a complication of antiretroviral therapy (ART). This study was done to look upon the effect of ART on CVD risk markers in patients on different ART regimens and comparing them with ART naïve patients.

Methods: It was a cross-sectional observational study done in 120 HIV infected individuals in a tertiary care centre in New Delhi. Cardiovascular risk markers were assessed and correlated with disease specific factors within individual subgroups differentiated as gp A (ART naïve), gp B (1st line ART) and gp C (2nd line ART). All cases with the past history of diabetes, hypertension, CVD, stroke or recent opportunistic infection (within last six months) were excluded. Carotid intimal medial thickness (CIMT) and high sensitivity c reactive proteins (hsCRP) were done to classify cases as having CVD.

Results: CVD risk parameters were found to be significantly higher in cases on ART as compared to ART naïve cases. Amongst cases who were on ART, these parameters were found to be significantly more in those on second line ART [i.e. protease inhibitor (PI) based regimens] as compared to those on first line ART, [i.e. non-nucleoside reverse transcriptase inhibitor (NNRTI) based regimens].

The mean CIMT amongst cases in gp C, gp B and gp A was 0.072±0.01cm, 0.063±0.01cm and 0.055±0.01cm respectively ($p<0.01$). 95%, 65% and 25% cases in gp C, gp B and gp A respectively had high CIMT (>0.06 cm)predicting high subclinical CVD. CIMT was seen to be directly correlated with disease related factors i.e. duration of disease ($p=0.02$), duration of ART ($p=0.01$), type of ART ($p=0.001$), low CD4 cell counts ($p=0.02$), along with classical risk factors i.e. fasting blood sugar ($p=0.04$), high triglyceride levels ($p=0.034$) microalbuminuria ($p=0.01$), hsCRP ($p=0.01$) and high waist hip ratio ($p=0.02$) respectively.

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Non Alcoholic Fatty Liver Disease And Metabolic Syndrome In Patients With Hiv/Aids And Its Correllation With Anti Retroviral Therapy And Severity Of Disease

Dr. Pulin K Gupta

Abstract

Introduction: Metabolic syndrome (MetS) and non alcoholic fatty liver disease (NAFLD) are a major cause of morbidity in chronic HIV infection associated with antiretroviral therapy (ART). This study was done by including HIV infected individuals and comparing antiretroviral therapy (ART) naive patients with patients on different ART regimen and evaluating the effect of ART on MetS and NAFLD.

Method: It was a cross-sectional observational study done on 120 HIV infected individuals in a tertiary care centre in New Delhi. All cases with hypertension, diabetes, chronic kidney or liver disease, thyroid disorders or on any drugs except ART were excluded. The risk markers for MetS were assessed and compared within groups on different ART regimens.

Results: Metabolic syndrome and NAFLD were found to be significantly more in cases on ART as compared to ART naïve cases. MetS was found to be associated with longer duration of disease (p=0.04), longer duration of ART (p=0.02) type of ART (protease inhibitors>NNRTI >no ART) and low CD4 cell counts (p=0.01). In those patients who were on ART, these parameters were found to be more in those on second line ART (i.e. protease inhibitor [PI] based regimens) as compared to those on first line ART, (i.e. nonnucleoside reverse transcriptase inhibitors [NNRTI] based regimen). 15% of cases on 2nd line ART (gp C) had MetS as compared to 12.5% in those on 1st line ART (gp B) and nil in ART naïve cases (gp A). One third (34%) of all 120 cases were found to have NAFLD. Significantly higher number of cases (45%) in gp C had NAFLD as compared to 32.5% in gp B and 25% in gp A respectively. Insulin resistance and metabolic risk markers were also significantly higher

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Exploring the Unique Usage of g-C_3N_4.SO_3H Ionic Liquid as an Efficient Catalyst for One-Pot Synthesis of Biologically Active 1,1-Dihomoarylmethane Scaffolds

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Abstract

1,1-dihomoarylmethane scaffolds possess several interesting physical and chemical properties, including high lipophilicity, good bioavailability, and the ability to form stable complexes with metal ions. These properties make them highly promising candidates for drug development, as they serve as a basis for the synthesis of bioactive molecules with potential therapeutic applications. They possess varied pharmacological activities namely anti-inflammatory, anticancer, and antimicrobial effects. Owing to the utmost significance of 1,1-dihomoarylmethane scaffolds, continuous efforts have been undertaken by the scientific community to develop practical, eco-friendly, and highly efficient approaches for their synthesis. In continuation, a highly promising approach has been developed for the synthesis of functionalized 1,1-dihomoarylmethane scaffolds using g-C_3N_4.SO_3H ionic liquid via Knoevenagel-Michael reaction. The method involved the reaction of C-H activated acids with a range of aromatic aldehydes, in a 2:1 ratio catalyzed by g-C_3N_4.SO_3H ionic liquid catalyst. The catalyst was synthesized from urea powder and chloro-sulfonic acid and was thoroughly characterized using FT-IR, XRD, SEM, and HRTEM studies. 1,1-dihomoarylmethane scaffolds were obtained with high yields, selectivity, and efficiency, using mild reaction conditions, no need for chromatographic separation, and short reaction times. Moreover, the approach adheres to green chemistry principles and also offers a viable alternative to the reported methods.

Keywords: 1,1-dihomoarylmethanes, green synthesis, g-C_3N_4.SO_3H, recyclability, gram-scale synthesis

Synthesis of 2-Aminothiazole Functionalized Imidazo[1,2-a]pyridines via Transition-Metal Free Approach as Novel Antibacterial Agents

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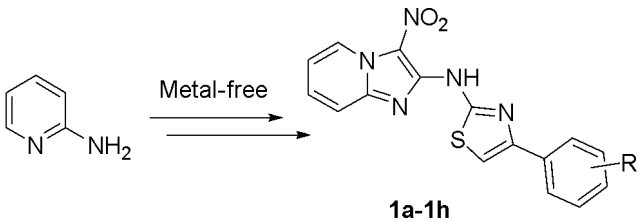
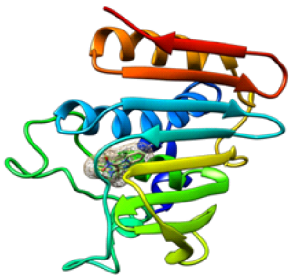
Abstract

The present work describe the synthesis, characterization and *in silico* studies of some new 2-aminothiazole functionalized imidazo[1,2-a]pyridines (**1a-h**). The key precursor **2** was synthesized by four steps method using 2-aminopyridine and chloroacetic acid as commercial available starting materials. The synthesized compounds **1a-1h** displayed considerable activity against Gram-positive bacteria. In particular, compound **1b** (R=2,4-dichloro) and **1e** (R=4-carbethoxy) exhibited significant activity against *S. aureus* and *B. subtilis* in comparison to standard antibacterial drug Ampicillin. The molecular docking and DFT studies of synthesized compounds were used to study the binding modes of these compounds. The compounds showed excellent binding energy scores (-8.3 to -9.3 kcal/mol) when interactions of 1KZN protein (*E. coli*) with compounds were examined which are in agreement with *in vivo* antibacterial activity.



1a-1h

R = 2,4-di-Cl (**b**)
4-$COOC_2H_5$ (**e**)



Interaction of **1e** with protein 1KZN (*E. coli*)

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Nucleophilic Sulphur and Amine-Enabled Assembling of S=C-S, S-N, Umpolung C-N, and C=C Bond formation in an Aqueous Medium

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Abstract

Unpredicted assembling of S=C-S, S-N, C-N, and C=C bonds in a row in natural solvent water to provide access to rarely found structural design is presented. Accordingly, the presented protocol paved the way for assembling multiple bond formation in a novel isothiazole-5-(2H)-thione with no catalyst, and additives with the divergent role of primary amine in aqueous medium.

***Keywords**:* Amine, Sulfur, Aqueous medium, Multiple bonds formation in a single step

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Keto Diet – Boon or Bane

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Abstract

Ketogenic diet is a normo-caloric diet composed of high fat, low carbohydrate and provides adequate calories. It includes a state of nutritional ketosis in which, under shortage of glucose, there is overproduction of ketone bodies which are used as a source of energy, especially in the CNS as it cannot use fat as an alternate source of energy. Ketogenic diet has been explored in various other conditions .Many active researches are underway to prove their role in other area as well. As of current knowledge, ketogenic diet has been proven to be beneficial in: Diabetes, Cardiovascular Disease, Obesity and Epilepsy. However, the benefit of ketogenic diet comes with certain risk like hypoglycemia, worsening renal functions , gut dysbiosis.

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POSTER ABSTRACTS

Study of 1,4-dihydropyridines Based Commercially Available Drugs

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Abstract

The exploration of novel N-containing heterocycles having potential biological and pharmacological properties have attracted immense interest in present era. Among them, 1,4- dihydropyridines have been recognized as versatile synthetic intermediates that provide access to variety of pharmacological active N-heterocycles. 1 Natural products containing 1,4- dihydropyridine ring can be used in pharmaceutical and agrochemical industries. 2 1,4- Dihydropyridine ring in biological system is significant as it occurs in reduced form of NADH (nicotinamide adenine dinucleotide) and NADPH (nicotinamide adenine dinucleotide phosphate). 1,4-Dihydropyridines are well explored scaffolds for binding with multiple receptors and possess several activities like calcium channel antagonists, antitumor, anti- inflammatory, antimicrobial, antihistamine, anticonvulsant, and analgesic. Commercially available drugs containing 1,4-dihydropyridine ring have been explored. The present study focuses on the various 1,4-dihydropyridine derivatives and their pharmacological actions. The important details about biological properties of 1,4- dihydropyridine would be more beneficial for the design and synthesis of more potent drugs.[4]

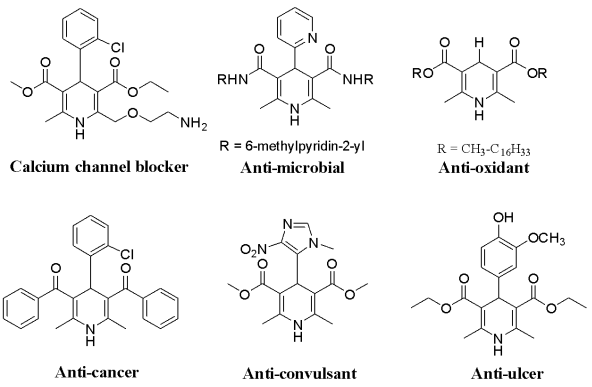

Figure 1. Commercially available drugs containing 1,4-dihydropyridine ring

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Antimicrobial Drug Resistance

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Abstract

One of the biggest risks to the world's public health this century is Antimicrobial resistance (AMR). Published in April 2014, the first Global Report on AMR surveillance by the World Health Organisation (WHO) gathered data from national and international surveillance networks for the first time, demonstrating the scope of the phenomenon in many regions of the world as well as the existence of significant gaps in the current surveillance. In this study, we concentrate on antibacterial resistance (ABR), which now stands in the way of both the high rates of resistance seen in common infections-causing bacteria and the intricacy of the consequences.Antimicrobial resistance is a major problem for international public health agencies. Nonetheless, new hospital and community-based data indicated a rise in the prevalence of antibiotic resistance in emerging nations like Bharat. It is extremely difficult to do research on the use of antibiotics, the causes and evolution of antibiotic resistance, regional variations, and interventional techniques tailored to the specific health care environment of each nation. The situational analysis of antimicrobial resistance is covered in this study, along with the solutions that will be needed in the future to lessen the problem's burden in Bharat. The writers gathered, examined, and analysed recent data from Medline, Google, and other sources. Studies conducted in hospitals revealed that resistance varies and is higher in some areas than others.In Bharat, studies on the public health implications of antimicrobial resistance at the community and hospital levels, as well as standard treatment guidelines, a national plan for containing AMR, and antimicrobial policy need to be developed and strengthened immediately.

Keywords: obstacles, antimicrobial resistance, Bharat, guidelines, surveillance, antibotics.

Tuberculosis: An Infectious Disease

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Abstract

Tuberculosis (TB) is one of the most ancient diseases of mankind, with molecular evidence going back to over 17,000 years. Despite newer modalities for diagnosis and treatment of TB, unfortunately, people are still suffering, and worldwide it is among the top 10 killer infectious diseases, second only to HIV. It is an airborne infectious disease caused by organisms of the Mycobacterium tuberculosis complex. Although primarily a pulmonary pathogen, M. tuberculosis can cause disease in almost any part of the body. It mainly affects the lungs, making pulmonary disease the most common presentation. Other commonly affected organ systems include the respiratory system, the gastrointestinal system, the skin, the central nervous system, the musculoskeletal system, the reproductive system, and the liver. It spreads through the air when infected people cough, sneeze or spit. Those who are infected but not (yet) ill with the disease cannot transmit it. TB disease is usually treated with antibiotics and can be fatal without treatment. The most common antibiotics used are streptomycin, rifampin, isoniazid, ethambutol.

Keywords: Tuberculosis, Mycobacterium tuberculosis, Antibiotics, Affected Areas

Gymnema Sylvestre In Diabetes Mellitus

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Abstract

Diabetes mellitus (DM) also known as hyperglycemia, is a chronic illness that is caused by a complex interplay of hereditary and/or environmental factors. The frequency of DM has increased dramatically over the last several decades in almost every nation, resulting in a "growing epidemic." Anti-diabetic activity of GS (Gymnema sylvestre) lies mainly in the leaf and is comparable to Metformin and Glimepiride. It is a promising plant for the treatment of Type 2 Diabetes Mellitus. It also shows anti-diabetic activity at lesser concentrations. Gymnemic acid is the main active chemical constituent isolated from the Gymnema Sylvestre plant. The plant is documented to possess beneficial effects as digestive, anti-inflammatory, diuretic, hypoglycemic, and antihelmintic. It is believed to be used in dyspepsia, constipation, jaundice, haemorrhoids, cardiopathy, asthma, bronchitis, and leucoderma. Gymnemic acids and gymnemasaponins are major chemical constituents of this plant and are classified as oleanane saponins. Gymnema Sylvestre possesses remarkable hypoglycemic properties and forms the platform of diabetes therapeutics in the traditional system of medication and thus can be used with their low cost and minimal side effects.

Keywords: Diabetes Mellitus, Gymnema sylvestre, gymnemic acid, gymnemasaponins, oleanane

Mosquito Ferritin and its Crucial Role in Iron Metabolism and Plasmodium Survival

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Abstract

Malaria remains a substantial and persistent global health challenge. There have been 249 million reported malaria cases for the year 2023, surpassing the pre pandemic levels according to WHO. The complexity of malaria is generally dependent on three factors i.e. the host(human), plasmodium and the vector (Anopheles mosquito). Vector is very crucial for disease propagation as plasmodium spends the maximum time of its life cycle inside the vector. Interestingly vector survival and disease progression are largely dependent on blood feeding and iron metabolism. However very little is known about the mechanism of iron metabolism by anopheles' mosquitoes, and my present work is dedicated to understanding this process in molecular details. My results clearly show that ferritin plays a very important role in the mosquito iron metabolism pathway. Ferritin is a ubiquitous cage-like protein, acting as a primary iron storage for almost all organisms. In the insect family they are also responsible for iron transport along with transferrin. While its function remains almost similar across different species, its structural complexity varies widely as we go down the evolutionary scale. Between a highly evolved mammal like human, to a primitive prokaryotes like bacteria, insects can be considered as an intermediary species in evolution. Mosquitoes are a unique group even within insects, due to their hematophagous nature and life cycle which goes from aquatic to air-borne. What makes mosquito ferritin even more interesting is its chimeric nature and its unique iron storage and transport properties. We found that ferritin expression is highly dependent (up-regulation) on mosquito diet (blood-meal ingestion), we also discovered that ferritin is transporting iron to ovaries and playing a crucial role in egg development. As ferritin plays a pivotal role in mosquito iron metabolism, we targeted ferritin at different stages of mosquito life-cycle by using ferritin selective and broad iron chelators, and the larvicidal effect was observed at even 15.6 ppm LD50.When the same iron chelators were used in adult female post-blood meals feeding, the no. of oocytes decreased significantly. In summary all our data suggests that ferritin plays a crucial role in mosquito iron metabolism, and it could be used as a potential insecticidal target. The other objective of this study is to explore how plasmodium sequesters iron from the mosquito for its survival, and in my presentation, I will showcase all our recent findings related to mosquito iron metabolism and its crosstalk to plasmodium.

Keywords: Ferritin chimera, iron metabolism pathway, iron chelator, larvicidal, ovicidal

Design, Synthesis, *In-Silico* ADME Prediction and Anticancer Screening of Novel 6-Substituted Sulphocoumarin Trizoles

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Abstract

The sulfocoumarin (1,2-benzoxathiine-2,2-dioxides) are the coumarin bioisosteres, which was reported first time in 2012 by Grandane A. *et.al* research group as a novel family of isoform-selective CA inhibitors that exhibit remarkable selectivity against cytosolic, widely distributed CAI and CAII isoforms as well as transmembrane, tumour related CAIX and CAXII.Sulfocoumarins can be defined as aromatic compounds with bicyclic ring (an endocyclic and an exocyclic one) containing three oxygen and one sulphur atoms. Their derivatives were reported to inhibit TrxR activity in cancer cells and act as prodrug inhibitors for human cancer-associated carbonic anhydrases (CAs) IX and XII.[1] Additionally, they've shown promise in effectively treating both sensitive and drug-resistant cancer cells. Triazoles are other 5 membered N-Heterocycles that has been widely utilized as precursors in the syntheses of biologically active systems such as anticancers, antimicrobials, antifungals and other cytotoxic active agents.Therefore, we envisioned to incorporate two privileged moieties propargyl of different phenol derivatives and 6-Azido Sulfocoumarin into a single one via Click Chemistry to form a Novel 6-Substituted Sulfocoumarin Trizoles for improved biological applications We have made a library of highly bioactive Triazole-Sulfocoumarin hybrids. The methodology involved in the synthesis of these hybrids is very simple. Use of cheap reagents, simpler reactions conditions and easier isolation of these hybrids with good yield percentage makes it more attractive.All the new synthesized compounds were characterized by various spectroscopic techniques (such as IR, NMR (^{1}H, ^{13}C), and mass spectroscopy). We will be discussing *In-silico* ADME Study [2] and anticancer activity of synthesized compounds[3].

***Keywords*:** Sulfocoumarin, Anticancer Activity, ADME Study, 1,2,3-trizoles, Click Chemistry

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Photocatalytic Degradation Of Azure-A in Aqueous Solutions Using Graphitic Carbon Nitride

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Abstract

The photocatalytic degradation of Azure-A was studied using graphitic carbon nitride (g-C_3N_4) as a photocatalyst. The effect of various parameters such as amount of catalyst, pH, light intensity and concentration of the dye has been studied on the rate of degradation. Kinetic studies revealed that this photocatalytic process followed pseudo-first order kinetics. A tentative mechanism for the photocatalytic degradation of Azure-A involving hydroxyl radical has been proposed.

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Neglected Tropical Disease

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Abstract

Neglected tropical diseases (NTDs) are a group of infectious diseases that primarily affect populations in low-income countries, particularly those living in impoverished conditions with limited access to healthcare. These diseases, such as malaria, dengue fever, and schistosomiasis, often thrive in tropical and subtropical regions, perpetuating a cycle of poverty and illness. Despite their significant impact on global health, NTDs have historically received little attention from the international community, leading to their designation as "neglected."This abstract examines the multifaceted challenges associated with NTDs, including inadequate funding, limited research and development initiatives, and social stigmatization. The consequences of neglecting these diseases are profound, with millions of people suffering from preventable disabilities, disfigurement, and even death. Moreover, NTDs exacerbate existing health disparities and hinder economic development in affected regions.Efforts to address NTDs have gained momentum in recent years, driven by increased awareness, collaborative partnerships, and innovative interventions. Global initiatives such as the World Health Organization's roadmap for NTDs and public-private partnerships have made significant strides in scaling up interventions, improving access to essential medicines, and enhancing surveillance and monitoring systems. However, sustaining progress against NTDs requires continued political commitment, resource mobilization, and community engagement. By prioritizing comprehensive and integrated approaches, the international community can effectively mitigate the burden of neglected tropical diseases, improve health outcomes, and advance towards achieving universal health coverage and sustainable development goals.

Keywords :- malaria,dengue fever,schistosomiasis, stigamtisation.

In-Silico Studies of Isatin Derivatives and Anti-inflammatory Activity

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Abstract

A physiological response to tissue destruction caused by microbial pathogen infection, chemical irritation, or injury is called inflammation. There is strong evidence linking inflammation to atherosclerosis, cancer, diabetes, arthritis, and Alzheimer's disease. Cyclooxygenase enzymes play a vital role in inflammatory conditions and have been classified into COX-1 and COX-2 isoforms. Anti-inflammatory drugs are always in high demand since they help to treat a variety of diseases, including cancer, heart disease, gout, osteoarthritis, Alzheimer's disease, and others, by acting as symptomatic treatments for inflammation and pain. Due to their harmful side effects, non-steroidal anti-inflammatory medicines (NSAIDs) have restricted applications. The most common side effect is gastrointestinal toxicity, which can occasionally coexist with ulcer, bleeding, or gastroduodenal perforation problems. Therefore, creating novel chemicals with increased potency and decreased toxicity is required. Isatin has demonstrated a unique biochemical profile, making it an attractive heterocyclic compound, and it has an indole nucleus. It has been reported that the Schiff and Mannich bases of isatin derivatives exhibit a range of pharmacological actions, including antimicrobial, antifungal, anticonvulsant, antidepressant, anti-HIV, and anti-inflammatory properties. Rational drug design benefits significantly from molecular docking research. Molecular docking studies are employed to precisely identify the different interactions that occur between ligands and enzyme active sites, which aids in the development of new, effective inhibitors. PDB ID-5KIR is the cox-2 receptor protein against which new isatin derivatives have been docked.

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Plant Tissue Culture and Its Application in Sustainable Development as Biotechnological Tool

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Abstract

Since ancient times trees have been an integral part of human life and a vital component of biodiversity. Forest trees are renewable sources of food, fodder, fuel wood, fiber, timber and other valuable non-timber products. Due to rapid deforestation, depletion of genetic resources coupled with escalating human needs the forest cover is being reduced tremendously from the earth's surface. Importance of forest cannot be underestimated. Recently rapid industrialization, urbanization and over-exploitation are the main factors of depletion of forest resources and permanent loss of forest.The worldwide demand for their numerous functions and outputs is increasing with the expanding population, while the global forest resource is shrinking as a result of overharvesting, deforestation and permanent conversion to other forms of land use in many regions. The regeneration of forest needs a certain period to maintain its sustainable function. Sustainable development can be defined as "economic development that meets the needs of the present without compromising the ability of future generations to meet their own needs". Traditional breeding methods are often constrained by the long reproductive cycles of most tree species and difficulty in achieving significant improvements to complex traits such a wood properties, disease and pest control, and tolerance of abiotic stresses. Plant Biotechnology is the application of science and technology to plants, parts, products and models to alter living or inert materials in order to develop knowledge, goods and services. In all the plant related biotechnologies, plant tissue culture has become an indispensable tool and a large number of methodologies have been exploited commercially. The emergence of modern method of plant tissue culture has provided a very alternative, which allows rapid propagation of desired plant species in a limited space under strict control of growth conditions. *In vitro* production of plants is generally described as micropropagation. This is one of the most important and commercially exploited areas where plant tissue culture has played a significant role. Micropropagation biotechnology has been recently applied in plantation forestry to derive huge economic benefits. Moreover, the biotechnological tools have allowed the genetic modification of forest tree species which can be used for reforestation and afforestation of degraded lands. A large number of plants of horticultural, floricultural and silvicultural importance have been successfully propagated.

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Exploring the Pharmacokinetics, Druglikeness, Antifungal and Antioxidant Potential: Synthesis and Characterization of Novel Alkyne-Azide Hybrids of 4,7-Dichloroquinoline

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Abstract

Quinoline is an active pharmacophore and is used as a therapeutic agent for various diseases such as malaria, tumour, and hyperpigmentation, and it has also possessed various other biological activities (antioxidant, antiplasmodial, antibacterial, antimicrobial etc). 4,7-Dichloroquinoline is an intermediate that leads to chemical modifications into less toxic, affordable and more effective drugs [1]. Our present study focuses on synthesising a targeted series of terminal alkyne and a novel azide derivative of 4,7-dichloroquinoline via copper-catalyzed cycloaddition (CuAAC) click chemistry also named Husigen's 1,3 dipolar cycloaddition resulting in the formation of triazole moiety with different substituents [2]. We checked their pharmacokinetics and drug-likeness using online software [3] and evaluated their antifungal and antioxidant potential. Their formation was proven by various spectroscopic techniques like Mass Spectrometry, Nuclear Magnetic Resonance Spectroscopy(^{1}H,^{13}C) and Infrared spectroscopy. The antioxidant activity was evaluated using ABTS (2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) assay [4] and the antifungal activity was done using antifungal strain i.e. *Aspergillus fumigatus*. We have effectively synthesized several novel 4,7-dichloroquinoline triazole hybrids and assessed their pharmacokinetic and drug-likeness characteristics, determining these compounds to be promising candidates for safe drug development. Additionally, we conducted evaluations to gauge their potent antifungal and antioxidant properties.

Keywords: Quinolines, Azide, Alkyne, Antioxidant, Anti-fungal, Spectroscopic techniques, Biological Evaluation.

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In-silico Studies of Phytoconstituents from Bael Leaves

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Abstract

According to the ancient scriptures, bael leaf i.e. the leaf of *Aegle marmelos* is known to heal every disease. The whole magic of curing and healing lies in its active constituents. The major constituents include aegelin, marmesinin, skimmianine, coumarins, phenylpropanoids, phenylethyl cinnamides, lupeol, beta-sitosterol, marmeline, flavones and citronellal. The pharmacological properties found in bael leaves are antioxidant, antispasmodic, antimicrobial, antitumor, etc [1].

So, I present in my work, the *in-silico* docking studies of the active constituents present in the leaves of *Aegle marmelos* against the receptors of certain diseases like diabetes, prostate carcinoma, inflammation, diahhorea, depression & anxiety, cardiac disorders and some more. The active constituents will be checked for different pharmacological activities and thus, we will get a summary about which constituent is responsible for that particular activity[2].

The software used for docking studies is AutoDock Tools 1.5.7 and visualization will be done through Biovia Discovery Studio. The *in-silico* studies of this plant will help the researchers to explore the future aspects of bael leaves and its utilization as a herbal remedy to cure ailments and to discover potent hybrids along with the minimization of toxicity and adverse drug reactions[3].

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Isatin and It's Derivatives: A Survey of Recent Synthesis, Reactions and Application

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Abstract

Isatin (1H-indole-2,3-dione) and its derivatives represent an important class of heterocyclic compounds that can be used as precursors for drug production.Isatin is a precursor for many synthesised therapeutic molecules that are amenable to pharmacological action.The isatin and its derivatives are used as bactericide, fungicide, anti-HIV, anti-epileptic, anti-instigative and so on.The isatin derivatives are helpful in inhibiting the activity of the urease and α-glucosidase enzymes and reduce the risks of pyelonephritis, gastric problems and diabetes. Due to its privileged scaffolding, the synthetic versatility of isatin has produced many structurally diverse derivatives, including the substitution of mono-, di- and tri- substitution of the aryl rings A and those derived by derivation of isatin nitrogen and C2 and C3 carbon moieties.So, improving and expediting access to isatin-related molecules is a challenging study in synthetic organic chemistry.

Keywords: Isatin, Heterocyclic compounds, Therapeutic, anti-epileptic, anti-instigative, enzymes,

In Silico Docking Studies of Coumarin Derivatives for their Potential Anti-Inflammatory Actions

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Abstract

Numerous studies have shown that coumarin derivatives block the lipoxygenase and cyclooxygenase pathways involved in arachidonate metabolism. In the current *in silico* study, 4-hydroxy coumarin derivatives were designed and docked against COX-2 receptor (PDB ID: 5F19) for their anti-inflammatory activity and the physiological parameters (ADME) were carried out by SwissADME software. 2D and 3D visualization of docking results were done by BIOVIA Discovery Studio. The results of the docking studies reveals that the designed 4-hydroxy coumarin derivatives are promising anti-inflammatory agents and these findings will be highly beneficial in optimizing the utility of coumarin derivatives in development of inflammation therapeutics.

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Antidiabetic Potential Of Developed Nano Lipid Carriers Loaded With Phytoconstituent: In Vitro And In Vitro Studies

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Abstract

Umbelliferone a pharmacologically active phytoconstituent has several pharmacological effects including antihyperglycemic activity. Constituents of umbelliferone are poorly water-soluble and low-permeable compounds, with consequently limited oral bioavailability. The present study aimed to prepare nano lipid carriers loaded with umbelliferone to overcome these issues. Nano lipid carriers were prepared by the melt emulsification method which was followed by sonication. The nanocarriers were characterized by DSC, FTIR, and TEM. The prepared nano lipid carriers have a significant entrapment efficiency of 85.47 ± 3.72%. The in-vitro release study showed a dual release pattern with early burst release followed by sustained drug release of 92% for 24 hours. Optimized formulation were evaluated in vivo for their anti-hyperglycemic potency towards type-II diabetes mellitus in rats. In-vivo studies revealed significant anti-diabetic effects after oral administration of nano lipid carriers to streptozotocin- nicotinamide-induced diabetic rats. The effect is assessed in terms of body weight, fasting blood glucose level, and various biochemical parameters. Umbelliferone-loaded nano lipid carriers had significant anti-diabetic effects even though they contained approximately one-quarter of the dosage relative to the pure form.

Keywords: Nano lipid carrier, umbelliferone, Bioavailability, Diabetes mellitus

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Docking Study of 1,3,4-Oxadiazole Derivative as Potent Analgesic

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Abstract

Oxadiazole is a heterocycle, five-member ring with one oxygen, two carbons, two nitrogen atoms, and two double bonds. 1,3,4-oxadiazole, Because of its many biological applications, the heterocyclic ring is one of the most significant heterocyclic moieties**.** This study highlights the use of 1,3,4-Oxadiazole derivatives as a potent analgesic agent. In this study the small designed library of 1,3,4-Oxadiazole derivatives were docked against COX-2 receptor (PDB ID:5F1A), and also physiological parameters were examined through SwissADME. According to the study of substituted oxadiazole revel that oxadiazole derivative possess analgesic activity.

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Development of Phytosomes by Solvent Evaporation Method and Its Evaluations

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Abstract

The object of present study is to develop and evaluate the phytosomes by ethanol based solvent evaporation method. Phytosomes are also known as phospholipid complex. It can be defined as phyto means plant and some means cell like. As dichloromethane, 1, 4 – dioxane, and tetrahydrofuran (THF) have been used as a choice of solvents for the preparation of stable phytosomes but these solvents have been found low solubility and precipitation problems during formation of phytosomes. Therefore, the solubility problem can overcome by using ethanol as a solvent choice because of its semi polar nature, class III solvent with a low toxicity profile and higher solubility of drug and lipid [1]. Chrysin was chosen as a model drug and phosphatidylcholine as lipid. The drug and lipid ratios were taken 1:1, 2:1, 1:2, and 2:2 (CP1, CP2, CP3 and CP4 respectively) as well as evaluation parameters of optimized formulation was done by Particle size, Zeta potential, Fourier transforms infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Differential Scanning calorimetery (DSC), in- vitro release study, fitted in kinetic models such as first order, zero order, Higuchi and Korsmeyer peppas. CP3 was optimized formulations and it was free flowing powder, percentage yield was 89% and extent of complexation was 87%. The characterization study of optimized formulation (CP3) was done by FTIR which showed there is no interaction between drug and lipid. The particle size and zeta potential obtained was 482.8 nm and -23.9 mv respectively. SEM study showed morphology of phytosomes which was spherical in shape. DSC study showed complete amorphization of chrysin by lipid and form stable complex. In-vitro release study of CP1 showed sustained release and followed Higuchi Kinetic model. The study showed that Phytosome is a promising drug delivery for enhancing the absorption of Phytoconstituents at gastrointestinal membrane and its bioavailability.

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Pharmacognostic And Physicochemical Analysis Of *Barleria Cristata* Linn.

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Abstract

The goal of the current study was to assess *Barleria cristata* Linn. Leaves Pharmacognostical characteristics and physicochemical analysis. As advised by the WHO, macroscopic, microscopic, and physicochemical investigations were conducted on variables such as moisture content, ash values, and extractive values.

The presence of calcium oxalate crystals, trichomes, vascular bundles, and stomata was identified by microscopic investigations. Established physicochemical properties, including ash content, extractive values, and moisture content.

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Breaking Barriers: Advancements and Challenges in Cancer Research and Treatment

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Abstract

Cancer, a complex and heterogeneous disease, continues to present formidable challenges to global health. Cancer in the broader sense refers to more than 277 different types of cancer disease. This review paper provides a comprehensive overview of recent advancements in cancer research and treatment modalities, highlighting breakthroughs in understanding the molecular mechanisms driving oncogenesis, as well as innovative diagnostic and therapeutic approaches. From the identification of novel cancer biomarkers to the development of precision medicine strategies, the paper explores the diverse landscape of cancer biology and clinical management. Additionally, it discusses emerging technologies such as immunotherapy, gene editing, and nanomedicine, which hold promise for revolutionizing cancer treatment paradigms. Furthermore, the paper addresses critical issues such as cancer disparities, drug resistance, and the integration of artificial intelligence in oncology practice. Through a synthesis of international research findings and expert perspectives, this review aims to provide a roadmap for future directions in cancer research and treatment, fostering collaboration and innovation in the global fight against cancer.

Keywords: Cancer, oncogenesis ,immunotherapy, nanomedicine, oncology

Improved Anti-Inflammatory Effects of Liposomal Astaxanthin on a Phthalic Anhydride-Induced Atopic Dermatitis Model

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Abstract

Background:
Atopic dermatitis (AD) is a common chronic inflammatory skin disease characterized by the mass release of cytokines. Stimulated keratinocytes release cytokines and chemokines associated with innate immunity, such as thymic stromal lymphopoietin (TSLP), interleukin (IL)-1b, IL-33, chemokine (C-C motif) ligand (CCL)17, and CCL22. Astaxanthin (AST) elicited an anti-inflammatory response in an experimental atopic dermatitis (AD) model. However, the use of AST was limited because of low bioavailability and solubility.

Methodology :
We hypothesized that liposome formulation of AST could improve AD. This study compared the anti-inflammatory and anti-dermatotic effects of liposomal AST (L-AST) and free AST. We evaluated the impact of L-AST on a phthalic anhydride (PA)-an induced animal model of AD by analyzing morphological and histopathological changes. We measured the mRNA levels of AD-related cytokines in skin tissue and immunoglobulin E concentrations in the serum. PA-induced dermatitis severity, epidermal thickening, and infiltration of mast cells in skin tissues were ameliorated by L-AST treatment.

Result:
L-AST suppressed AD-related inflammatory mediators and the inflammation markers, inducible nitric oxide synthase (iNOS) and cyclooxygenase (COX)-2 in PA-induced skin conditions. Oxidative stress and expression of antioxidant proteins, glutathione peroxidase-1 (GPx-1) and heme oxygenase-1 (HO-1), were recovered by L-AST treatment in skin tissues from PA-induced mice. L-AST treatment reduced transcriptional activity of STAT3 and NF-kB in PA-induced skin tissues.

Conclusion:
Our results indicate that L-AST could be more effective than free AST for AD therapy

***Keywords**:* Astaxanthin, liposome, atopic dermatitis, oxidative stress.

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"ALLIUM STRACHEY" the Endangered and Traditional Medicinally Important Herb of Uttarakhand Himalaya, Bharat

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Abstract

Allium stracheyi (jumboghass) is an endangered and ethnobotanically important herb with high medicinal value in the Uttarakhand Himalaya. It is a perennial, small herb, up to 35 cm tall, and is commonly grown in Jammu Kashmir, Himachal Pradesh, Uttarakhand, Nepal, and Pakistan at elevations of 2500-3625 m. A. stracheyi is used as traditional vegetables and has been included in the Red Data Book of Bharatn plants due to its indiscriminate collection and resulting threat to its existence. The plant has been identified as having sulfur-containing oil, which has antioxidant, anti-inflammatory, and antimicrobial properties. It is also reported to reduce blood cholesterol. A. stracheyi contains various biologically active compounds, including phenolic acids, flavonoids, thiosulfinates, alkaloids, fixed oils, phytosterols, and sulfur-containing compounds. Its nutritional value includes protein, fat, fiber, carbohydrates, calcium, phosphorus, iron, magnesium, and potassium per 100 mg. The plant contains volatile and sulfur-containing compounds, including hydrocarbons, terpenes, and terpenoid. The volatile compounds, such as (Z,Z,Z)-9,12,15-octadecatrienoic acid, have been reported to have anti-inflammatory and antioxidant properties, anxiolytic-like effects, and relief in spasmodic and arthritic pain.

Keywords *:* Allium stracheyi, photochemistry, pharmacological application, sulfur contents, traditional importance.

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Membrane-Active Hydantoin Derivative as Anticonvulsant Agents

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Abstract

One of the most valuable resources available to humanity at all ages and activity levels is brain health. The brain health is disturbed by several neurological disorders, and the major neurological disorder of epilepsy is one of them. My poster presentation addresses the effect of the anticonvulsant drug on epileptic patients and the docking studies of newly prepared anticonvulsant derivatives which show better ADME properties and docking scores in comparison to marketed drugs. Which can be further useful as anticonvulsant drugs if all the testing procedures are cleared. Yet through docking studies found that its protein binding is better than the standard drug phenytoin. Anticonvulsant drugs are highly neurotoxic which causes several side effects, so there is a need to design derivatives with less neurotoxic effects that would be useful for the patient, so the moto of my study is to develop a less neurotoxic derivative of hydantoin where I compared standard drugs dock score with designed analogs, ADME properties and physiological properties by AutoDock, Swiss ADME software.

***Keywords*:** anticonvulsant, docking, phenytoin, designed analogues.

In-Silico Studies Of Phenyl/Imino Piperazine Derivatives Against Depression

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Abstract

Depression is a chronic mental disorder that affects up to 20% of people worldwide. A piperazine is a six-membered heterocyclic ring that has two opposing nitrogen atoms and is used for various therapeutic activities including depression. The phenyl/imino piperazine derivatives have a potent antidepressant effect. They showed great potential in *in silico* studies and proved to be good mono-amino oxidase inhibitors. In this study, various phenyl/imino piperazine derivatives were designed and docked at the respective active sites of the receptor using various docking softwares (autodock vina, pyrax etc.) and was evaluated for their drug likeness (using the software SwissADME) and bioactivity scores (using the software Molinspiration). The derivatives showed good docking and bioactivity scores and displayed drug-like characteristics, including blood-brain barrier permeability. Thus, these derivatives can be further synthesized and carried out for in vivo evaluation to show potent anti-depressant activity.

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Computational Assessment of the Toxicological Profiles of the Degradation Products of the COVID-19 Drug Paxlovid

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Abstract

The idea of safe-by-design, or SbD, must be taken into consideration when creating and using a drug or when people may be exposed to the drug's metabolites or degradation products. It encompasses safe waste management, safe design, safe production, and safe usage of new materials and technology. Pfizer's innovative antiviral medication "Paxlovid" and it is a good COVID-19 medication. The drug is marketed under the brand name PaxlovidTM and is composed of two generic drugs: ritonavir and nirmatrelvir. The safety profile of the medication as well as their metabolites and degradation products should be determined. Within this study, we have performed the computational assessment of toxicological effects on human health and the environment of Paxlovid and its degradation products. Because computational studies may anticipate biological effects and toxicity profiles and correlate them with structural and physicochemical attributes, they may be a useful tool in evaluating the safe design of chemicals. Here we have used different types of computational tools such as SwissADME, PreADMET, admetSAR2.0, CarcinoPred-EL, Pred-hERG, ENDOCRINE DISRUPTOME, ProTox-II, Pred-Skin, ADMETlab2.0 and other related computational tools for the assessment of different types of toxicities. The major findings are the drug and its degradation products have very low metabolizing enzyme inhibition activity, almost no central nervous system activity, very low mutagenicity, carcinogenicity, cytotoxicity, and immunotoxicity, very weak potential of cardiotoxicity, and no skin-sensitizing activity, very low hepatic and nephron toxicity but it may cause serious respiratory, reproductive and mitochondrial toxicity. It shows moderate Fish aquatic toxicity. To maximize the drug's safety profile, these findings may be utilized to supplement or direct the current in vitro and in vivo toxicity testing.

***Keywords**:* Paxlovid, safe-by-design (SbD), computational tools, toxicity testing

In-silico Study of Phytochemicals Fused with Benzimidazole Ring for COX-2 Inhibition: Potential Drug Target Against Inflammatory Disease

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Abstract

Since the ancient time, herbs are used as curing agent. Based on traditional knowledge and practices, it is widely used. With the use of modern synthetic medicine, the use of herbal medicine had been cut down but in present it regained its popularity. As per WHO 80% OF people use herbal medicine in primitive healthcare. Herbal formulations are widely accepted therapeutic agents as antidiabetic, antiarthritic, hepatoprotective. Diclofenac sodium is one of the important medicines prescribing for arthritis patients since last 25 years. But this drug is also the limitations of gastrointestinal adverse effects associated with the traditional non- selective NSAIDs. It was studied that free –COOH group responsible for GI toxicity of these NSAIDs. The especial structural features of benzimidazole and a wide range of biological activities of its derivatives made it prosperous structure in drug discovery. At this time, benzimidazole scaffold has emerged as a pharmacophore for choice of designing analgesic and anti-inflammatory agents active on different clinically approved targets. Benzimidazoles got an increased attention due to their outstanding bioavailability, stability and important biological efficiency. The main objective of this work was to synthesize novel compounds with a Benzimidazole scaffold by Piperazine as a building block. Molecular docking was done in the COX-2 active site to predict the possible binding mode and rationalize the structure–activity relationship of the synthesized compounds. The main causes of numerous Non-Steroidal Anti-inflammatory Drugs (NSAIDs), Drug induced gastrointestinal ulceration, renal side effects and hepatotoxicity are. Cyclooxygenase-2 (COX-2) inhibitors found to decrease the gastrointestinal issues, but woefully, most of them are associated with major cardiovascular adverse effects. In this study, molecular docking investigations of outlined derivatives were done utilizing Protein Data Bank (PDB ID-2AW1). Most of the compounds indicated high scores as compared to standard during molecular modelling, analysis and displayed interactions with active amino acids of a COX-2 enzyme. role in binding with the COX-2.

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Biogenesis, Isolation, and Application of Cow Milk-derived Exosomes

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Abstract

Exosomes (EXOs) are naturally occurring endosome-derived nanoparticle that are released by several biological cells. Earlier exosomes were thought to be merely the waste products from maturing red blood cells therefore they did not receive much attention at that time. Exosomes are now found in all body fluids including plasma, urine, tears, cerebral spinal fluid, semen, bronchial fluid, saliva, serum, amniotic fluid, synovial fluid, lymph, gastric acid, bile, breast milk. The only biological liquid with EXOs that is produced commercially is milk. Exosomes have their beginnings in endosomes ,and the ultimate content of the exosomes is produced as a result of interaction with various intracellular vesicles and organelles during the biogenesis process. They have the same traits as their parents and can be derived from several sources. Size exclusion chromatography, density gradient centrifugation, or (ultra) centrifugation can be used to separate EXOs from milk; however, however, because of the complex makeup of milk, which includes casein micelles and milk fat globules , there are additional consideration that must be made when using the aforementioned methods on milk. In addition to these benefits, exosomes prolong their usefulness as delivery vehicles by preventing undesired buildup or by homing to the liver, which avoids metabolic problems. These organic carriers have extended circulation times and can transport therapeutic loads that can even breach the blood brain barrier, posing some serious therapeutic problems.

Keywords*:* Exosomes, Cow milk, biogenesis, isolation technique, application

Fullerene

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Abstract

It seems like you're referring to "fullerene," a molecule composed entirely of carbon, often in the form of a hollow sphere, ellipsoid, or tube. Common examples include buckyballs (C60) and carbon nanotubes. How can I assist you with fullerene. Fullerenes, such as C60, have a spherical structure composed of 60 carbon atoms arranged in a pattern of 12 pentagons and 20 hexagons, resembling a soccer ball. The carbon atoms form a cage-like structure with alternating single and double bonds. This arrangement gives fullerenes unique properties and has implications in various fields like materials science and nanotechnology.

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Linking Pesticides to the Onset and Progression of Cancer

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Abstract

To eradicate pests, chemical compounds known as pesticides are employed. In addition to pests, nontarget organisms are also at risk from them. They release reactive oxygen species (ROS), which can impede various enzymes and receptors, hence causing disruption to cellular activities. Analysing epidemiological evidence regarding the connection between chemical pesticides and cancer. Numerous pesticides have been demonstrated in animal trials to induce cancer, including sulfallate, organochlorines, and creosote. Organochlorines, such as DDT, lindane, and chlordane, are known to stimulate tumour growth. Certain contaminants included in commercial pesticide formulations have the potential to cause cancer. The International Agency for Research on Cancer has classified pesticides and arsenic-containing compounds used in the workplace as human carcinogens. Exposure to these chemicals can disrupt cell function and DNA integrity, causing genetic mutations and damage. Some pesticides, called carcinogens, can directly transform healthy cells into cancerous cells by causing DNA mutations or stimulating cell growth. In addition, long-term use of antibiotics can weaken the immune system and make it less able to identify and eliminate cancer cells, thus promoting Cancer. The relationship between pesticides and cancer highlights the importance of strict control and safety measures in the use of pesticides to protect human health.

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Enzyme catalyst

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Abstract

They are typically proteins with specific three-dimensional structures that enable them to bind to substrates and facilitate reactions, often by lowering the activation energy required for the reaction to occur. Enzymes play crucial roles in various biological processes, such as digestion, metabolism, and cell signaling. Enzyme catalysts find diverse applications in various industries. Some notable examples include:

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Role of Nanotechnology to Combat Environmental Pollution

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Abstract

Chemistry plays a multifaceted role in combating pollution by creating technologies, materials and processes that reduce the impact of pollutants on environment and human health. Chemical reactions are used to synthesize nanoparticles and nano materials allowing researchers to tailor the properties for specific purposes such as catalysis, drug discovery and environmental remediation.The present study experimentally investigated the effect of Nanotechnology to combat environment pollution by offering innovative technologies that can remove pollutants,enhance energy efficiency and monitor environmental conditions like:

- Magnetic Nanoparticles can be used in water treatment to remove contaminants.
- Nano catalysts accelerate the production of biogas.
- Nano sensors aid in real time monitoring of pollution levels.
- Nano membranes with finest pore size can be used to capture and separate particulate matter and gases in the atmosphere.

Overall, with precautions Nanotechnology offers promising tools to address and mitigate environmental pollution.

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4-Chloroquinolin-2(1H)-one Derivatives a Source of New Antimalarial

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Abstract

A potentially fatal disease, malaria is carried on by Plasmodium-genus protozoan parasites. More than 249 million fatal cases of this disease were reported in 2022 alone, making it one of the leading causes of death worldwide. Spread via bite of infected female Anopheles mosquitoes, these parasites have a complex, multistage life cycle in their mosquito vector and vertebrate hosts. The major factor contributing to the resurgence of malaria includes the formation of drug-resistant strains of malaria, spreading of insecticide- resistant strains of mosquito and also the lack of licensed malaria vaccines of proven efficacy. 1 Among the known five strains of malaria, P. falciparum is the primary cause of malarial fatalities that might also lead to death among young children in the regions of Asia and Africa. 2 4,7-dichloroquinoline is a known anti-malarial lead compound, similar to it is 2,4-dicholoroquinoline derivatives that are found in many biologically active compounds known to show anti- malarial properties. In this presentation we will discuss the synthesis of 2,4-dicholoroquinoline and its derivatives. Further we will discuss the future aspect of our lead molecule in terms of novelty and the activity in different malarial P. falciparum cell line.

***Keyword*:** 4-Chloroquinolin-2(1H)-one, Anti-malarial, P. falciparum

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Heterocyclic Fragments and Enhanced Anticancer Properties

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Abstract

Heterocyclic compounds are defined by IUPAC as "cyclic compounds having as ring members atoms of at least two different elements". Naturally occurring heterocycles seem to be vital for biochemical reactions in the metabolism of cells. By 2015, approximately 30% of the FDA-approved anticancer drugs and medicines were having one or more cyclic rings which have nitrogen and oxygen. Our main focus is towards the activity of heterocyclic compounds as anticancer agents. Few of the Heterocyclic drug names approved by FDA for their anti-tumor properties are Xalkori(Late-stage Non-small-cell lung carcinoma (NSCLC)), Caprelsa (Metastatic medullary thyroid cancer),etc.The vast array of heterocyclic structures found in biological systems, such as co-factors, nucleic acids, and proteins, form the foundation of heterocycle engineering and rational design. Even their ease of modification with additional substituents indicates that these are great options to start when developing anti-cancer medications. Strategies for nanovectorization are a viable solution that offer improved biocompatibility through passive targeting and increased permeability and retention impact. There are lesser short-comings of such heterocyclic compounds based drugs compared to other available drugs and also their promising effect as anti cancer agent is really impressive. Here, we broadly discussed the use of heterocyclic compounds as anticancer agents,various drugs based on heterocyclic compounds and their importance, their structural activity relationship, impact on human body and the advantages of using Nanovectorization strategies.

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Innovations in Drug Discovery: Advancing Therapeutics for Heart Diseases with a Focus on Cardiac Arrest

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Abstract

Cardiac arrest, a sudden and life-threatening event, remains a leading cause of mortality globally. This abstract provides an insight into recent advancements in drug discovery aimed at revolutionizing the treatment and prevention of heart diseases, with a particular emphasis on addressing the complexities of cardiac arrest. Understanding the intricate molecular and cellular mechanisms underlying cardiac arrest is crucial for the development of targeted therapeutic interventions. The poster presentation will explore the latest breakthroughs in drug discovery, highlighting novel compounds that show promise in mitigating the risks and consequences associated with cardiac arrest. Key areas of focus will include the identification of pharmacological agents designed to modulate ion channels, enhance myocardial contractility, and optimize coronary perfusion. Furthermore, the integration of cutting-edge technologies such as precision medicine and gene therapy into drug development will be discussed, emphasizing their potential in tailoring treatments to individual patients based on their genetic predispositions and specific risk factors. The presentation will also shed light on emerging pharmaceutical strategies aimed at promoting cardiac resilience, addressing the aftermath of cardiac arrest, and preventing subsequent complications. This encompasses the exploration of drugs that facilitate tissue repair, reduce inflammation, and improve overall cardiac function in the post-arrest phase. In conclusion, the poster aims to provide a comprehensive overview of recent drug discoveries in the realm of heart diseases, with a particular focus on advancements pertaining to cardiac arrest. By delving into the molecular intricacies and technological innovations driving these discoveries, we aim to contribute to the ongoing efforts to enhance therapeutic options and outcomes for individuals at risk of or affected by cardiac arrest.

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Chorea: Unraveling the Dance of Neural Dysfunction and Exploring the Therapeutic Avenues

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Abstract

Chorea, a neurological disorder characterized by involuntary, rapid, and unpredictable movements, poses a significant challenge to both patients and healthcare professionals. This abstract provides an overview of chorea, highlighting its clinical manifestations, underlying etiology, and the current understanding of its pathophysiology. Chorea can manifest as a primary feature of Huntington's disease, a hereditary condition, or secondary to various other neurological and metabolic disorders. The impact of chorea on the quality of life of affected individuals is substantial, emphasizing the need for effective therapeutic interventions. This poster presentation aims to explore the pharmacological approaches employed in managing chorea. Traditional treatments have included drugs such as neuroleptics, benzodiazepines, and tetrabenazine. However, advancements in our understanding of the molecular mechanisms involved in chorea have led to the development of more targeted and efficacious therapies. The presentation will delve into the emerging role of drugs that modulate neurotransmitters, particularly dopamine, which plays a pivotal role in the pathogenesis of chorea. Novel medications, including dopamine receptor antagonists and inhibitors, will be discussed, shedding light on their mechanisms of action and potential benefits in chorea management. Additionally, the poster will touch upon the importance of a multidisciplinary approach in chorea treatment, incorporating physical therapy, occupational therapy, and psychological support to enhance overall patient well-being. In conclusion, this poster presentation aims to provide a comprehensive understanding of chorea, its impact on individuals, and the evolving landscape of drug interventions. By exploring current and emerging pharmacological strategies, we hope to contribute to the collective knowledge base and foster advancements in the therapeutic management of this intriguing movement disorder.

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Adsorption of Cd(II), Cr(II), Cu(II), Pb(II) and Zn(II) Ions from Ultramarine Blue Industrial Effluents by *Colocasia esculenta* (arbi peels) as Low-Cost Adsorbents

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Abstract

The ability of arbi peels, *colocasia esculenta* was investigated as low-cost natural adsorbents for adsorptive removal of Cd(II) Cu(II), Cr(II), Pb(II) and Zn(II) ions from ultramarine blue industrial effluents (aqueous solutions). Different physico-chemical parameters were studied such as pH, adsorbent dose, equilibrium contact time, and metal ions concentration. Thermodynamic parameters were also evaluated, which indicated that this adsorption process was not only physisorption but also there was some chemisorption.

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Linking Pesticides to the Onset and Progression of Cancer

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Abstract

To eradicate pests, chemical compounds known as pesticides are employed. In addition to pests, nontarget organisms are also at risk from them. They release reactive oxygen species (ROS), which can impede various enzymes and receptors, hence causing disruption to cellular activities. Analysing epidemiological evidence regarding the connection between chemical pesticides and cancer. Numerous pesticides have been demonstrated in animal trials to induce cancer, including sulfallate, organochlorines, and creosote. Organochlorines, such as DDT, lindane, and chlordane, are known to stimulate tumour growth. Certain contaminants included in commercial pesticide formulations have the potential to cause cancer. The International Agency for Research on Cancer has classified pesticides and arsenic-containing compounds used in the workplace as human carcinogens. Exposure to these chemicals can disrupt cell function and DNA integrity, causing genetic mutations and damage. Some pesticides, called carcinogens, can directly transform healthy cells into cancerous cells by causing DNA mutations or stimulating cell growth. In addition, long-term use of antibiotics can weaken the immune system and make it less able to identify and eliminate cancer cells, thus promoting Cancer. The relationship between pesticides and cancer highlights the importance of strict control and safety measures in the use of pesticides to protect human health.

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Exploring Surface and Secretory Proteins of Plasmodium Falciparum as Diagnostic Markers

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Abstract

Malaria presents a significant health challenge in most tropical countries, and its diagnosis is a crucial pillar in the control and elimination efforts, often accomplished by the administration of mass-scale Rapid diagnostic tests (RDTs). Rapid diagnostic tests (RDTs) for malaria are considered cost-effective and user friendly which detect the presence of HRP2 antigen (histidine-rich protein 2) in patient blood samples. The inherent limitations of RDTs are insensitivity in scenarios of low transmission settings and deletions in Plasmodium *falciparum* hrp*2/3 (*pfhrp2/3*)* proteins and single nucleotide polymorphisms (SNPs), thus necessitating the need to explore new novel diagnostic tools/targets. Previously our group employed Peptide Microarray technology to screen immunoreactivity of cyclic constrained peptides from thirteen antigenic proteins (CSP, EXP1, LSA1, TRAP, AARP, AMA1, GLURP, MSP1, MSP2, MSP3, MSP4, P48/45, HAP2) of Plasmodium *falciparum*. Cyclic peptides (C6, A8, B7- cyclic constrained) and (G11, DSQ, NQN- corresponding linear peptides) were compared for their immunoreactivity against P. *falciparum* infected sera. However, three cyclic constrained immunoreactive peptides- C6:Exported Protein1(EXP1), A8:Merozoite surface protein (MSP2), B7:Glutamate rich protein (GLURP) demonstrated highest immunoreactivity with field samples. However, these peptides required further validation for development of specific antibody based new rapid diagnostic tests. To achieve this, we recombinantly expressed these target proteins *i.e.* Exported Protein1(EXP-1) and Glutamate rich protein (GLURP) and generated polyclonal antibodies. We are now in the process of quantitating the secretion of these target proteins from in vitro P. *falciparum* culture, as well as from field samples.

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Infectious Disease and Global Health

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Abstract

Infectious diseases are a significant global health concern, posing threats to populations around the world. These diseases, caused by pathogens such as bacteria, viruses. parasites, and fungi, have the potential to spread rapidly and cause widespread illness and death. HIVI-AIDS, tuberculosis, malaria, influenza, and COVID-19 are among the key infectious diseases that have garnered attention due to their impact on public health and economies. The burden of these diseases is particularty high in low- and middle-income countries, where access to healthcare and resources for prevention and treatment may be limited. Additonaly, emerging infectious diseases, such as Ebola and Zika virus, continue to challenge global health security. Efforts to address infectious diseases and promote global health require a multifaceted approach. This includes robust surveilance systems to monitor disease spread, vaccination programs to prevent infections, access to affordable and effective treatments, and public health interventions to control outbreaks. Furthermore, collaboration between govemnments international organizations, healthcare providers, researchers, and communities is essential for coordinating responses, sharing resources and expertise, and implementing evidence-based strategies to reduce the burden of infectious diseases and protect public health on a global scale.

Keywords: Infectious diseases, global health, pathogens, HIV/AIDS, tuberculosis, malaria influenza, COVID-19, low- and middle-income countries, public health, emerging infectious diseases, surveillance, vaccination, treatments, interventions, collaboration, governments international organizations, healthcare providers, researchers, communities, responses, resources, expertise, strategies, burden.

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Modulation of Host Response by Plasmodium During Liver Stage Development: A Strategy to Survive.

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Abstract

In sub-Saharan Africa and South-East Asia, malaria caused by Plasmodium sp. infection is still one of the most common infectious diseases and is endemic. In order for the parasite to invade and replicate in hepatocytes, a number of host components are necessary during the parasite's mandatory asymptomatic hepatic stage of infection. In addition to being potential therapeutic targets for treating drug-resistant malaria, many genes of the parasite and the host are essential to parasite invasion and survival tactics. [1]. We have chosen 5 genes- CPS1, PTGS1, KLF6, KLF4, and SOC3 which were found to be up-regulated in the early stages of the Plasmodium life cycle in the hepatocytes, according to Transcriptome analysis. [2]

We employed siRNA to systematically examine the related genes in human HepG2 cells for their potential functions during infection by *P. berghei* sporozoites in order to determine how host cell signal transduction pathways affect hepatocyte infection. [3]

The significant down regulation of our selected 5 genes were analysed by qPCR and a staggering 90% reduction was observed compared to the control which was not treated by any siRNA. We tried to transfect the HepG2 cells with siRNAs to down regulate the expression of these 5 genes and found out an increase in the sporozoite invasion when cultured in-vitro.

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"Click Chemistry" Approach Towards The Synthesis of Ethynlestradiol Based Radiopharmaceuticals as Potential Breast Tumor Imaging Agents

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Abstract

Estrogen receptors (ER) are expressed in very high numbers in the breast cancer cell lines and hence, **ER** is considered as an ideal biomarker for the molecular targeting of breast cancer [1]. This work highlights the use of a new Ethynylestradiol based ER targeting ligand for its use in PET imaging and preclinical evaluation of breast cancer [2]. The research work focuses on the design, click synthesis, spectroscopic characterization, and preliminary biological evaluation of Ethynylestradiol (EE2) functionalized macrocyclic chelating agent DOTA-EA-Triazole-EE2. The ligand has been synthesized via the reliable and efficient class of Cu(I) catalyzed azide-alkyne cycloaddition in quantitative yield. The ligand has been spectroscopically characterized and the in-vitro cytotoxicity profile of the ligand has been assessed on HEK and HeLa cell lines.The MTT results exhibit 90% cell survival after 72 h incubation of HEK and HeLa cells with different concentrations of DOTA-EA-Triazole-EE2 construct.The in-vitro cytotoxicity studies exhibit the safe and biocompatible nature of the developed ligand. Further in-vitro biological studies are in progress. We are optimistic that the synthesized PET agent will exhibit improved stability, affinity, efficacy, and safety profiles over the existing probes and can be successfully extended from bench to clinic after successful in vivo studies. This type of study will also pave way for the development of other promising ligands in the fields ranging from in vitro diagnostics to in vivo molecular imaging of breast cancer.

Keywords: PET, radiopharmaceuticals, breast tumor, imaging

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Annulene and it's Properties

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Abstract

Annulene is a cyclic hydrocarbon with alternating single and double bonds, belonging to the larger class of annulenes. The most well-known annulene is benzene, a six-membered ring with three double bonds. Annulenes exhibit aromatic properties and have interesting electronic structures. The general structure of annulenes involves a cyclic arrangement of carbon atoms with alternating single and double bonds. The number of carbon atoms in the ring determines the size of the annulene. For example, benzene, a common annulene, has six carbon atoms in the ring.

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Calcium Channel Blockers

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Calcium channel blockers are drugs used to lower blood pressure. They work by slowing the movement of calcium into the cells of the heart and blood vessel walls, which makes it easier for the heart to pump and widens blood vessels. As a result, the heart doesn't have to work as hard, and blood pressure lowers. Potential side effects from taking a calcium channel blocker includes Dizziness or lightheadedness, Low blood pressure, Heart rhythm problems, Dry mouth, Edema (swelling of ankles, feet, or lower legs), Headache, Nausea, Fatigue, Skin rash, Constipation or diarrhea, Gastroesophageal reflux disease (GERD). Property of nondihydropyridines can be modified by altering the functional groups or altering the structure of molecules.

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Exploring Dipeptide Inhibitors for Plasmodium Falciparum Enoyl-Acyl Carrier Protein Reductase (PfENR): Molecular Docking and Dynamics Based Approach

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Abstract

Malaria, a life-threatening disease transmitted by infected female Anopheles mosquitoes, is caused by parasites of the Plasmodium genus[1]. Drug resistance in malarial strains has compromised the effectiveness of current treatments, necessitating the development of new drugs[2]. Targeting fatty acids synthesis in the liver and blood stage is crucial in combating P. falciparum. Plasmodium falciparum enoyl-acyl carrier protein reductase (PfENR) is a crucial enzyme involved in fatty acid biosynthesis[3]. In this study, we employed in-silico methods to identify potential dipeptide inhibitors for the PfENR enzyme. Virtual screening of a dipeptide library revealed Trp-Trp, Trp-Phe, Trp-Tyr, and Tyr-Phe as dipeptides with strong affinity towards PfENR. Molecular dynamics simulations were conducted to ensure the stability of protein-ligand complexes. Further analysis using Density Functional Theory (DFT) elucidated the electronic structure and reactivity of these dipeptides. Lead dipeptides were synthesized using solid-phase peptide synthesis, and characterized via LCMS. Our results indicate that dipeptides hold promise as PfENR inhibitors, offering valuable insights into combating malaria and potentially leading to a new class of antimalarials.

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A Metal Free Synthesis of enantiopure 2,3-dideoxy-α, β-unsaturated Carbohydrate enals

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Abstract

A metal free synthesis of enantiopure 2,3-dideoxy-α, β-unsaturated carbohydrate enals (Perlin aldehydes), in CH_3CN-0.02 N H_2SO_4 in water (1:1, v/v) with 0.5 equivalent additives (4-hydroxy-6-methyl-2-pyrone or 4-amino coumarin), has been reported [1]. This efficient protocol works well for the acetylated glycals (glucal, galactal and arabinal) and afforded Perlin aldehydes and hemiacetals in acceptable to good yields. Whereas, benzylated glycals furnished respective Perlin aldehydes, hemiacetals and the 2-deoxy derivatives, under similar reaction conditions. The products yields were significantly reduced when the additives were removed from the reaction mixture, indicating that they constitute an essential component of this approach. Further the use of 0.02 N H_2SO_4 in water: acetonitrile (1:1, v/v) solvent system is essential for the formation of Perlin aldehydes. The similar reactions under neutral reaction conditions (CH_3CN:H_2O, 1:1, v/v) with additives, afforded the hemiacetals as major product. This methodology is a metal free approach to Perlin aldehyde synthesis and therefore having additional benefit of its use as compare to previously reported methods [2-6].

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Understanding the Effect of Arsenic and Environmental Factors in Gallbladder Cancer

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Abstract

Gallbladder cancer incidence has surged in recent time in Bharat, notably in arsenic hotspots. Often diagnosed in advanced stages, the exact cause is unknown, but factors like gallstones increase the risk. Exposure to pesticides and arsenic contamination in Bihar's groundwater is associated with an increased incidence of gallbladder cancer. This study aims to establish an association between arsenic, pesticide exposure and gallbladder carcinogenesis. It involved the participation of 30 individuals serving as control volunteers and an additional 30 individuals with confirmed cases of gallbladder cancer. Biological samples, including gallbladder tissue, gallbladder stone, bile, blood, and hair, were collected from GBC patients for arsenic and pesticide estimation. Additionally, blood samples from 30 gallbladder cancer patients were evaluated for arsenic presence to understand the exposure level in the population. A significantly high arsenic concentration was observed in the blood samples of GBC cases, reaching a maximum of 141 µg/L compared to controls. Similarly, gallbladder cancer patients exhibited significantly elevated arsenic concentrations in gallbladder tissue (highest concentration of 182 µg/kg), gallbladder stones (192 µg/kg), and hair samples (510 µg/kg). The study of blood samples from 30 gallbladder cancer patients revealed a very significant arsenic concentration in the population of Bihar, with a maximum arsenic concentration of 141 µg/L. Arsenic concentration in biological samples was notably high in the arsenic-exposed area, indicating a substantial gallbladder disease burden in Bihar. Furthermore, environmental sample analysis, including water, rice, pulse, and vegetables, showed a high arsenic concentration of 912 micrograms in food samples. Pesticide analysis identified carcinogenic compounds like acetonitrile, tetrahydrofuran, and Aziridine, and other pesticides which may directly or indirectly contribute to gallbladder cancer development. The findings underscore a strong link between arsenic contamination, environmental exposure, and increased gallbladder carcinogenesis in Bihar.

Keywords: Gallbladder cancer, Arsenic, Environmental factors, Genetic factors

Ferrocene

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Abstract

Ferrocene is an organometallic compound with a unique sandwich-like structure, featuring a central iron atom between two cyclopentadienyl anions. It's known for its stability and has applications in catalysis and as a precursor in organic synthesis. Ferrocene has a distinctive structure with a central iron (Fe) atom sandwiched between two cyclopentadienyl (C5H5) rings. The overall molecular formula is (C5H5)2Fe. This arrangement forms a symmetric, planar, and stable molecule.

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Design and Synthesis of Peptides Targeting Plasmodium Proteins

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Abstract

Malaria poses a threat to world health causing estimated 247 million cases of malaria and over 619,000 deaths[1] . Drug-resistant parasites have emerged, highlighting the need for designing and development of new class of drugs in the ongoing battle to end malaria. Peptide-based medications have a high degree of specificity for intracellular targets, they represent a novel and promising therapeutics for malaria[2]. Plasmepsin II (Plm II) is an essential enzyme of P. falciparum involved in hemoglobin degradation pathway. In the present study, in-silico methodologies were used to identify the peptide based inhibitors for Plm II[3]. A virtual library of 400 dipeptides was generated and screened against Plm II. Pymol and Discovery Studio Visualizer were used for determining the interactions between the protein and the inhibitors. Specific and active penta-peptides were further designed by multiple overlapping of lead dipeptides based on substrate binding site. Two Penta-peptides (P1&P2) were finally selected based on their binding affinity -7.7 &-8.5 Kcal/mol respectively. Further, Penta-peptides were synthesized using Solid Phase Peptide Synthesis (SPPS) and were characterized using Mass Spectrometry.

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ICP-MS: An Analytical Aspect to Identify Heavy Metals and Minerals in Food Matrices

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Abstract

In recent years, the food industry has witnessed advancements in analytical techniques, which focused to enhance food safety and quality assurance. Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is a powerful and versatile tool in this context. This abstract gives an overview of the applications of ICP-MS in food safety, highlighting its important role in detecting and quantifying trace elements, heavy metals, and contaminants in food matrices. This technique helps in the identification of emerging food safety concerns, such as the presence of heavy metals, which may contaminate food products. ICP-MS can provide valuable inputs into the characterization and quantification of these emerging contaminants. The abstract gives an idea about applications of ICP-MS in food safety. It identifies the detection of heavy metals such as lead, cadmium, and mercury, highlights ICP-MS's ability to measure these contaminants at ultra-low concentrations. Furthermore, it explores the assessment of nutritional elements, such as essential minerals and vitamins. The role of ICP-MS in ensuring that food products meet recommended dietary allowances. Furthermore, ICP-MS plays a vital role in monitoring food contaminants by enabling the detection of ultra-low concentrations. Its versatility extends to the analysis of isotopic compositions, facilitating the tracing of food origins and authenticity verification, which is essential for preventing food fraud and ensuring product quality. In conclusion, ICP-MS has revolutionized the field of food safety by providing a robust, sensitive, and versatile analytical aspect for the detection, quantification, and characterization of elements and contaminants in food products. Its applications extend from regulatory compliance to nutritional assessment, ensuring that consumers can enjoy safe, authentic, and nutritious food which meets the highest standards of quality and safety in the food industry.

Keywords: ICP-MS, food safety, heavy metals, minerals, identification.

Case Study for Glaucoma

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Abstract

A 73-year-old female housewife presented with chief complaints of headache and loss of vision in one eye. The patient informed about decreased vision in one eye for the last two years. She also had undergone chemotherapy 3 years ago for treatment of breast cancer and also had IOL implantation in her right eye.

On examination, her vitals were normal except that her BP was higher. We also conducted an MRI of her orbit in which we found-

- Diffused thinning of the left optic nerve involving all segments, no evidence for compressive lesion
- Extraocular muscles appeared normal
- The right optic nerve was also normal in the course

MRI of her brain was also done which showed age-related diffuse cerebral and cerebellar atrophy. Her visual acuity for her right eye was 6/18 and her left eye had a loss of light perception.

The patient's blood sugar was 108mg/dl and homocysteine was 26.4 umol/L

So, our final diagnosis was that she was suffering from age-related primary open-angle glaucoma.

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Design and Characterization of Bilayer Herbo-Synthetic Tablet Dosage Form Containing Aloe-Vera, a Herbal Component as an Immediate Release Layer and Aspirin as a Sustained Release Layer

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Abstract

The present study is aimed to formulate, optimize and evaluate the Bilayer tablet of Aspirin and Aloe-Vera gel powder. Aspirin is a derivative of salicylic acid, and it used to reduce fever, pain, swelling in conditions such as arthritis but the major side effect is stomach bleeding and ulceration. Aloe Vera is a natural anti-ulcer agent and it helpful clinically in the management of peptic ulcers. As a consequence, the objective of the present work is to design a bilayer tablet of Aspirin as a sustained-release portion and Aloe-Vera gel powder formulated as immediate as release portion to prepare a single tablet containing two different drugs having a different category. In general sustained release drug delivery is attempted to maintained constant, effective drug level in the body with associated minimization of undesired side effects and herbal immediate-release layer release quickly and prevents the side effects that occur because of aspirin.

The pre-formulation study was carried out in order to identify the compatibility between drug and excipient/polymer by FTIR spectroscopy, DSC analysis and XRD analysis, results shown that drug was compatible to excipient without any significant changes in chemical nature of drug.

Development of the bilayer tablet of Aspirin and Aloe Vera gel powder was carried out in two different stages. Blends of sustained release of Aspirin and immediate release of Aloe Vera gel powder was done by 3^2factorial designs varying the concentration of excipients. Tablet layer was manufactured separately using 8 station compression machine and evaluated for their performance and effect of variables in formulation. After optimization of individual layer, the bilayer tablet was prepare using optimized formulas and evaluated. In- vivo study of optimized batch was also performed for the anti-ulcer activity.

Keywords: - Aspirin, Aloe Vera gel powder, optimization Bilayer tablet, sustained release, Immediate release.

Photocatalytic Degradation of Some Pesticides by Using Cerium Doped Zinc Oxide

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Abstract

Bispyribac-Na is Bispyribac-sodium is used as a broad spectrum post-emergent herbicide for the control of grasses, sedges and broad leaf weeds in rice crops. The photocatalytic degradation of Bispyribac-Na was observed in presence of Ce-doped zinc oxide (CZO) (photocatalyst). It was found that 3% Ce-doped ZnO could effectively degrade (78 to 86%) 30 µg/mL concentration of Bispyribac-Na in water in 7 hours. The Ce doped ZnO nanocrystalline powder was prepared by spiking of different Ce concentration (2-4%) in ZnO at high temperature (750˚C). This as-prepared Ce-doped photocatalyst was characterized by X-ray diffraction (XRD) or scanning electron microscope (SEM).

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Deciphering Dysregulated MYC and its Links with Metabolic Genes in Breast Cancer

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Abstract

Breast cancer represents a significant global health burden, with varying incidence rates observed across different regions of the world. it emerged as the foremost cause of global cancer incidence in 2020, with an estimated 2.3 million new cases, constituting 11.7% of all cancer occurrences. A complex process of MYC to the uptake of nutrients to make ATP is also an essential building blocks that increase cellular growth activates DNA replication, and causes cell division [1]. Glycolysis plays a significant role in the advancement of breast cancer and lessens the body's susceptibility to radiation and chemotherapy. The current study uses a variety of in-silico approaches to discover MYC's relationship with the major metabolic genes in patient datasets for breast cancer from different datasets, to evaluate expression [2]. We examined the expression and correlation between energy metabolism and MYC dysregulation by analyzing data from 250 breast cancer patients along with control samples from various databases, including TCGA. Employing in silico methods, we investigated MYC expression and its association with key metabolic genes such as HK-II, SLC2A1 (GLUT1), SLC16A1 (MCT1), PFKFB3, and lactate dehydrogenase-A. Our collective results shed light on the interplay between MYC expression and metabolic signaling in breast cancer [3]. Also, we validated and checked this study through Immunohistochemistry (IHC) of 28 Breast cancer tissue samples and found higher expression of MYC. Since, increased glycolysis has emerged as a major hallmark for cancer cell proliferation, targeting MYC could bring an impact to inhibit Breast Cancer progression. In order to reduce the glycolytic effects, this study explores the therapeutic potential of targeting MYC receptors in breast cancer.

Keywords: *MYC*, Metabolic gene, Hexokinase, Glycolysis, *In-Silico,* Immunohistochemistry

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Design and Development of Point of care device for Early Detection of Endometrial Cancer

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Abstract

The most common gynecological cancer in the western countries is endometrial cancer, and incidence rates are growing in lockstep with the obesity pandemic. Early identification is essential to improve survival, which is less than 20% in cases of advanced cancer and over 90% in cases of early-stage disease at 5 years. There are currently no biological markers that have been demonstrated by science to be early warning signs of it. There are currently no biological indicators that have been proven to be effective for its early identification. Advances in high throughput technologies and machine learning techniques now offer unique and promising perspectives for biomarker discovery, especially through the integration of genomic, transcriptomic, proteomic, metabolomic and imaging data. Because the proteome closely mirrors the dynamic state of cells, tissues and organisms, proteomics has great potential to deliver clinically relevant biomarkers for cancer diagnosis. Here, we present the current progress in endometrial cancer diagnostic biomarker discovery using proteomics approaches. We describe the various mass spectrometry-based approaches and highlight the challenges inherent in biomarker discovery studies. We suggest novel strategies for endometrial cancer detection exploiting biologically important protein biomarkers and set the scene for future directions in endometrial cancer biomarker research.

Keywords: endometrial cancer, diagnostic biomarkers, proteomics, mass spectrometry.

Pyrimidine Derivatives: Simulation, In Silico Parameterization, and Computational Application

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Abstract

Drug discovery have been using computational tools and in silico models to predict ADMET (Adsorption, Distribution, Metabolism, Excretion, and Toxicity) profiles of molecules, primarily to prevent late-stage failures caused by underprivileged pharmacokinetics and toxicity. Hence utilizing the ADMET Predictor generated data for synthesized cyclopenta[d]pyrimidine derivatives which leads with unique capabilities for discovery PK assessment and deployment before going in-vitro and in-vivo assessment. In order to further support fidelity and transparency in cyclopenta[d]pyrimidine derivatives optimization for drug development and the chemical sciences, established ADMET predictor learning models directly train on molecular pairs and their property differences. This model helps to develop the physiochemical property, metabolite stability, CYP450 isoenzyme inhibition, followed by metabolite identification and characterization of phase I and phase II enzymes. This allows the models to predict cyclopenta[d]pyrimidine derivatives properties accurately by processing individual derivative as inputs for biological, chemical, or physical properties. Conclusion of the characteristics of cyclopenta[d]pyrimidine derivatives increasingly frequently, as they allow for the assessment of larger candidate populations using computational modeling and simulation (PBPK) to identify and mitigate risks, this abstract will offer a basic stratagem to follow while transitioning from synthesis of larger candidate populations to preclinical.

Keywords: Cyclopenta[d]pyrimidine, ADMET; Absorption, distribution, metabolism, excretion, and toxicity Molecular Simulation, PBPK; Physiological based pharmacokinetic modeling and simulation

Synthesis and Characterization of Chalcones Containing 3-(Trifluoromethyl)-5-Amino Pyrazoles & Substituted Acetophenones

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Abstract

5-Chloro-3-(trifluoromethyl)-1-(4-substituted phenyl)-1H-pyrazole-4-carbaldehyde was prepared with the help of well-known Vilsmeier–Haack reaction with 3-(trifluoromethyl)-1-(4-substituted phenyl)-1H-pyrazole-5-one.5-Amino-3-(trifluoromethyl)-1-(4-substituted phenyl)-1H-pyrazole-4-carbaldehydes was prepared by nucleophilic displacement of the chloro group at C5 in 5-chloro-3-(trifluoromethyl)-1-(4-substituted phenyl)-1H-pyrazole-4-carbaldehydes with different amines in refluxing appropriate solvent using mild base. Aldehydes and substituted acetophenones were subjected to reaction at room temperature with ethanolic sodium hydroxide as base in order to prepare the pyrazolic chalcones. The structures of prepared compounds were confirmed by spectral data such as IR, 1H NMR, 13C NMR, and mass spectra.

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Immunomodulatory And Anticancer Activity of Plant Derived Chemicals Using *In-Vivo* Models in Albino Wistar Rats and *In-Vitro* Model Using Human Breast And Colon Cancer Cell Lines

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Background: Evaluation of preclinical immunomodulatory anticancer models are very crucial in the process of drug discovery and development. Dysfunctional immune system is linked with disorders like autoimmune diseases, inflammatory diseases, cancer and as a treatment immunosuppressive or immunostimulant drugs are prescribed aiming at immune system disease. Literature states that plants carry phytochemicals which exerts various biological activity in humans, mainly anti-inflammatory and anti-cancer properties which are likely to overcome the side effects caused by synthetic drug treatments.

Objective: To screen the ethanolic extracts of selected three medicinal plants – CP, MC, CO and combination (COMB) of above three plants (CP+MC+CO) for *in-vivo* and *in-vitro* immunomodulatory anticancer activity to cause a total effect of extracts (combination) higher than the sum of single effect of each extract.

Methodology: The extracts of selected plants (whole plant extract) were prepared by using maceration technique using ethanol as a solvent. The extracts were subjected for **1.** *In-vivo* immunomodulatory models – macrophage phagocytosis by carbon clearance test; T and B cell mediated immunity by Delayed Type Hypersensitivity test and Haemagglutination antibody titre in albino wistar rats based on acute oral toxicity tests. **2.** *In-vitro* anticancer potential using Sulforhodamine B (SRB) assay against breast and colon cancer cell lines at concentrations of 10, 20, 40 and 80 µg/ml.

Results: The extracts have shown effects on cellular and humoral mediated immunity thus confirming its immunomodulatory potential. All the extracts inhibited percent control growth in dose dependent manner for both breast and colon cancer cell line.

Conclusion: The combination of selected three medicinal extracts was exerting synergistic effects to modulate immune system and could be further explored for future studies. Optimization in experimental conditions or turning extracts into novel drug delivery systems can enhance the medicinal effects of the plants and can reduce the GI50 concentration considering the phenolic/flavonoid content richness of these plants.

Keywords: Immunomodulatory, anticancer, extracts, synergism, cellular and humoral immunity

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Synthesis of Ayurvedic Loha Bhasma (Powder)

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Abstract

Pure iron powder was taken as a starting material to synthesize Loha Bhasma in powder form and further purification was followed by use of different herbal juice treatments to soften malleability of the metal. After herbal treatment known multiple incinerations were given at higher temperature (600^0C) in natural Putta Bhatti (red fire). This Loha Bhasma is very useful in treating iron deficiency, Anemia. Loha powder is initially treated with juice of Ficus *amplissima* (Pimpri), banana leaves extract and Triphala decoction to soften the Loha metal and to remove impurities from it. This herbal juices treatments is known as bhavana. The preparation of Loha Bhasmas followed step by step; shodhan, special shodhan and marana. Process of maran was carried out at 600^0C and 800^0C to compare the quality of two products. The Bhasma formed at 600^0C was found in proper colour and meeting all quality parameters than prepared at 800^0C. Advanced analytical instruments tools were used to evaluate the quality of Loha Bhasmas such as ICP-OES, FTIR, and XRD.

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Green Methods of Synthesizing Chalcone: A Review

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Abstract

Chalcones are important scaffolds in the field of medicinal chemistry due to the presence of α, β-unsaturated ketone functionality. These are prepared by treating an aldehyde with acetophenone in the presence of an acid or a base using the Claisen-Schmidt condensation reaction. Numerous chalcone derivatives have been reported due to the their biological activity that has clinical implications for a range of disorders. The chalcones and their derivatives are synthesized by various eco-friendly methods such as the use of green catalysts and solvents, ultrasonic radiation, microwave energy, and methodologies involving grinding in the absence of solvents (mechanochemical method). Currently, green chemistry plays an important role in organic synthesis. It minimizes adverse effects on the environment and human health. The main goal of green chemistry is to use green solvents such as water, acetone, alcohol, etc. to eliminate the toxicity, uses of small quantity of catalyst and minimize the chemical accident during the process. So it is more effective to pharmacists or chemists in manufacture of desired compounds in a green manner. Green chemistry is also known as sustainable chemistry. For synthesis using green chemistry, there have been many criteria or methods that should be followed during manufacturing condition such as safer solvents, less hazardous chemical syntheses, avoiding waste, designing safer chemicals, design for more energy efficient chemical, use of renewable feed stocks, atom economy, reduce undesired derivatization, catalysis, design for degradation, real time analysis for pollution prevention, inherently safer for accident prevention, etc. So green chemistry provides a route of organic synthesis, and offers important environmental and economic benefits over traditional synthetic processes.

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Photocatalytic Degradation of Low Density Polyethylene (Ldpe) Using CaO Nanoparticles as a Catalyst

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Abstract

The photocatalytic degradation of low density polyethylene (LDPE) was carried out using CaO nanoparticles as a catalyst. After exposure, morphology as well as thermal properties of the specimen was investigated by scanning electron microscopy (SEM) and differential scanning calorimeter (DSC). Results before and after photodegradation of LDPE indicated that linear LDPE is much more prone to cracking into small snippet, giving rise to crystallinity with different amount of CaO nanoparticles. The DSC results confirmed a remarkable influence of photodegradation on degree of crystallinity (X_C %), fusion enthalpy (ΔH Jg^{-1}) and melting temperature (T_m) of LDPE. It was observed that LDPE was degraded successfully during photocatalytic conditions on using CaO nanoparticles.

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Floating Drug Delivery System: An Introduction or Review

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Abstract

The purpose of writing this review on floating drug delivery systems (FDDS) was to compile the recent literature with special focus on the types of floating drug delivery systems, principal and mechanism of floatation to achieve gastric retention. The main goal of any drug delivery system is to achieve desired concentration of the drug in blood or tissue, which is therapeutically effective and non-toxic for a prolonged period. Drug delivery systems are those that float immediately upon contact with gastric fluids present promising approaches for increasing the bioavailability of drugs with absorption in upper small intestine. The gastric emptying of a dosage form is a complex process and one of the biggest hindrance in the better absorption and increases bioavailability of oral drug delivery system. They provide an efficient means for improving the drug bioavailability; reducing drug wastage and better patient compliance by increasing the gastric residence time and provide controlled drug delivery. This review article is in pursuit of giving detailed information on the pharmaceutical basis of their design, classification, advantages and different types of FDDS and the future potential of FDDS.

Keywords: Floating Drug Delivery System, gastric retention, bioavailability

Biogenic Synthesis of Nickel Oxide using Rose Petal Extract and it's Photocatalytic Activity

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Abstract

In this study Nickel oxide nanoparticles (NiO NPs) were synthesised using rose flower extracts (RFE). The corrosion inhibition efficiency of the synthesized NiO NPs, was evaluated by electrochemical (EIS and PDP) tests. The XRD analysis of NiO NPs that showed single-crystalline characteristics. These nanoparticles were created in an environmentally friendly and cost-effective manner. This NiO NPs using RFE have been use in study of degradation of different dyes.

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Effect of *Trichoderma harzianum* on Growth and Yield of Corn and Tomato Under Water Stress

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Abstract

Drought is the major abiotic stress which has been increased over the past decades affecting world's food security. One possibility to increase the drought tolerance is to use beneficial microorganisms as seed inoculants. The filamentous fungal genus*Trichoderma*the most common occurring fungus in soil and has the ability to colonize and multiply in various habitats. *Trichoderma hargianum* are extensively used for biotic and abiotic stress management, crop growth enhancers. In this experiment the seed treatment with *Trichoderma harzianum*on the growth and productivity of Tomato (Solanum lycopersicum L.) Corn (*Zea mays* L.) under water stress conditionhas been tested.Pot experiments for both the cropshas conducted in randomized design with four replications in greenhouse condition. *Trichoderma harzianum* treated seeds are sown in each pot. Water stress started 15 days after sowing in water stress treatments and regulated watering is done in irrigated condition treatments and untreated control. In water stress treatments watering stopped for subsequent days until the plants attaining physiological wilting stages due to drought exposure and water is provided only after the appearance of wilting and leaf rolling symptoms due to physiological stress by providing water with the help of measuring cylinder. This watering method adopted till the end of the experiment.Suitable untreated controls used as reference for drawing conclusion while comparing the effect of *Trichoderma spp.* Incorporation of *Trichoderma* during seed biopriming treatmentsin corn and tomato has resulted in improved vegetative growth and yield performance in water stress condition. The seed treatment with *Trichoderma harzianum.* is comparatively easy, cost effective and ecofriendly practice for the farmers and good alternatives for chemical pesticides, PGR and fertilizers & safe for environment/ecosystem.

Keywords: Drought , stress , productivity, Trichoderma, corn, tomato

A novel approach to construct thiacalix[4]arene-appended coumarin based light-emitting supramolecular system for liquid crystalline and self-assembly behavior

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Abstract

A novel supramolecular system based onthiacalix[4]arene linked with coumarinwas designed and synthesized by esterification method, incorporating with different alkoxy side chains. All four supramolecular compounds exhibited nematic type liquid crystalline properties. The liquid crystalline properties and thermal stability of the compounds were studied by polarizing optical microscope, differential scanning calorimetry, and thermogravimetry analysis. Additionally, these materials demonstrated enantiotropictype mesophase with a wide temperature range and good thermal stability. Notably, they exhibited light-emitting properties in both solution and solid thin film states, showing the intriguing aggregation-induced emission effect. The selected compound was utilized to stain nematode samples using a solution-state aggregation approach. The fluorescent supramolecules effectively allowed visualization and tracking of staining patterns within the nematode organisms. This innovative staining methodology enabled the examination of cellular and subcellular structures, offering valuable insights into the behavior and morphology of nematodes.

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Analytical Method Development And Validation Of Amlodipine Drug By Different Analytical Techniques

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Abstract

Hypertension is a long-term medical condition, where the blood pressure in the arteries is persistently elevated. It is major risk factor for stroke, coronary artery disease, heart failure, atrial fibrillation, peripheral artery disease, vision loss, chronic kidney disease, and dementia. Hypertension is a major cause of premature death and affects 1 in 3 adults worldwide. Who report shows that approximately 4 out of every 5 people with hypertension are not adequately treated, but if countries can scale up coverage, 7,60,00,000 deaths could be averted between 2023 and 2050. The objecctive of present work is to develop and progressively validate a novel, simple, rapid, sensitive, economic and reproducible reverse phase HPLC method, which may reduce solvent ratio and cost also. The devloped method is easy to perform quickly without negative influence, and plot of LOD and LOQ chart plotted was linear with a regression coefficient of $R^2 > 0.999$.

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Photo-Degradation of Organic Dyes Using Binary and Ternary Graphene Oxide Composites: A Comparative Study.

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Abstract

The extents of industrialization causes serious problem of water pollution and large amount of pollutants such as dyes and organic solvents are discharged into water bodies which leads to a shortage of fresh and usable water which pose a serious threat to human health and the environment, that is why new technologies have been developed for the photo-degradation of organic pollutants. Graphene oxide have gained increasing attention because it possesses higher surface area, active functional groups, better electron transfer, improved thermal stability, improve dispersibility in water and easy to be incorporated with other materials to form binary and ternary composites. From the past ten years, ternary composites have attracted enormous interest over binary composites as binary composites are not so efficient for the degradation of organic dyes. Therefore, In the present investigation a comparative study of binary and ternary graphene oxide composites have been done on photo-degradation of organic dyes using various parameters such as effect of pH, effect of concentration of dyes, effect of amount of composites and effect of light intensity. It has been observed that more than 70% of the dye degraded in 90 mins. using ternary graphene oxide composite whereas in case of binary composite the percentage degradation of the dye is very low. Therefore, it has been concluded that ternary graphene oxide has the potential to be an efficient adaptable composite for the photo-degradation of organic dyes in industrial wastewater as compared to binary composites.

Keywords: Binary composites, Ternary composites, Graphene oxide, Organic dyes and industrial waste water.

Pandemic Preparedness and Response

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Abstract

In recent years there has been a global push for reliable pandemic preparedness indicators. Example: In response to the COVID-19 pandemic, several international initiatives have been developed to strengthen and reform the global architecture for pandemic preparedness and response, including proposals for a pandemic treaty, a Pandemic Fund, and mechanisms for equitable access to medical counter measures. the importance of robust primary health care in equitably and efficiently safeguarding communities from future health threats. The international community should not repeat the mistakes of past health security efforts that ultimately contributed to the rapid spread of the COVID-19. This Health Policy paper outlines major (although often neglected) gaps in pandemic preparedness and response, which are applicable to broader health emergency preparedness and response efforts, and identifies opportunities to reconceptualise health security by scaling up universal health coverage. This is vital given the current drive to include social and governance metrics in revised efforts at data collection, as well as efforts to include pandemic preparedness indicators to improve or help in the development of pandemic preparedness and response. This review aim to provide tangible solutions that equitably meet the needs of all communities while ensuring resilience to future pandemic threats.

Keywords: Pandemic, COVID-19, pandemic treaty, health emergency

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Oxidation of Benzyl Alcohols by Molecular Oxygen Catalyzed by Cobalt Ferrite

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Abstract

Oxidation of alcohols to aldehydes/ketones/carboxylic acids is an especially crucial step in organic synthesis. Normally, strong oxidants oxidize alcohol to carboxylic acid and this reaction may or may not stop at the intermediate steps like aldehyde and ketone. Some mild oxidants are required to stop it here at this stage. Here, molecular oxygen enters the scene, which can help in achieving this objective, but there is a disadvantage to use molecular oxygen as an oxidant as it has a slow rate of oxidation. Hence, such a reaction may be catalyzed by metal ferrites. These metal ferrites are easy to separate by using an external magnet and can be recycled. Cobalt ferrite has been used for the oxidation of benzyl alcohols to corresponding benzaldehydes.

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Photocatalytic Reduction Of Carbon Dioxide To Fossil Fuel By Using Tungsten Doped Titanium Dioxide Powder

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Abstract

Photocatalytic reduction of carbon dioxide into fossil fuel or hydrocarbon-containing material in presence of sunlight is important from environment point of view. The W doped titanium dioxide powder was synthesized via hydrothermal method. It was obtained in nanocrystalline state. The structural pattern of W doped titanium dioxide was investigated by field emission scanning electron microscopy (FESEM), energy dispersive X-Ray analysis and X-Ray diffraction data. It was observed that photocatalytic CO_2 reduction over W doped titanium dioxide was higher as compared to TiO_2. Formic acid and formaldehyde were identified as photoproducts. The progress of reaction was monitored spectrophotometrically using cromotropic acid (CTA). The effect of the variation parameters such as concentration of carbon dioxide, amount of photocatalyst, light intensity and pH on the yields of photoproduct was also optimised.

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Physico-chemical, Spectral, and Antimicrobial Evaluation of New substituted benzaldehydes derivatives of Pyrrolo [2, 3-d]-Pyrimidinehydrazide Bearing Azomethine Moiety

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Abstract

New substituted benzaldehyde derivatives of pyrrolopyrimidinehydrazide bearing a biologically active azomethine moiety were synthesized, characterized (solubility, stability, melting points), spectral studied (PMR, UV, and FT-IR spectra), and tested for antimicrobial activity. The antibacterial and antifungal activities of the synthesized compounds were demonstrated by MIC values varying from 50 to 250 g/mL. *Staphylococcus aureus* MCC 2010 was the most resistant, while *Escherichia coli* MCC 2412 and *Pseudomonas aeruginosa* MCC 2080 were the most susceptible. The antimicrobial screening results revealed that all of the tested compounds have considerable activity, with some being found to be more active than the reference drugs used. (*streptomycin* and *fluconazole*).

Keywords: Pyrrolopyrimidinehydrazide, Azomethine, Antimicrobial screening, Antifungal activities

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Liquid Chromatography-Mass Spectrometry (LC-MS/MS) Mycotoxins in Food Analysis

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Abstract

Mycotoxins are natural food toxins reproduced by certain fungi developed on different crops during pre-harvesting and post-harvesting conditions. During testing, selection and extraction of sample taken after by clean-up is an primary process for accurate and final detection. These steps give ensured the accuracy, precision as well as the reliability, and reproducibility of testing results. It can be used to detect various mycotoxins with accuracy and precision. Therefore, the review has focused on the co-occurrence, masked mycotoxins, sampling, the extraction of mycotoxins, and LC–MS/MS as an analytical tool for the accurate and precise detection mycotoxins. The extraction of mycotoxins from liquid samples like milk, wine, juices, is be done using mostly liquid–liquid extraction (LLE) and in solid samples like cereals, dry fruits, spices, feed, a solid–liquid extraction process have adopted. Mycotoxin comes from the Greek term 'mykes' and 'toxicum', 'meaning' fungus/mold and poison . The production of these toxins occurs under certain conditions such as moisture content, temperature, food matrix. These mycotoxins are entered the human body through the direct use of contaminated food, or ingestion food from plants, or indirectly food obtained from the animal source such as eggs, meat, and milk . Mycotoxins have appeared hazardous impacts on the human body. Mycotoxins affects on humans includes change in genome expression, kidney failure, disease of the reproductive system and intestinal tract and cancer in the body. The presence of mycotoxins in food and food products is a serious matter, and it affects the health of consumers and the country's economy. The presence of mycotoxins in food is a severe problem that affects the quality and safety of food and affects consumers' health.

Keywords-, Food Safety, Mycotoxins, Electrospray Ionization.

Parkinsons Disease: A Neurological Disorder

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Abstract

Parkinson's disease is the most common progressive neurodegenerative disorder affecting older adults all over the world. More than 6 million Worldwide have Parkinsons' disease. It happens due to the lack of Dopamine. Dopamine deficiency in the basal ganglia leads to classical Parkinsonian motor symptoms; viz, bradykinesia, tremor, rigidity, and later postural instability. The diagnosis is clinical and sometimes difficult, considering the large number of motor and non-motor symptoms in PD patients. Parkinson's disease can't be cured, but medicines can help to control the symptoms, often dramatically. Levodopa, the most effective Parkinson's disease medicine is a natural chemical that passes into the brain and is converted to dopamine.

***Keywords*:** Parkinson's disease, a neurodegenerative disorder, dopamine, levodopa.

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Photocatalytic Removal of Congo Red in Presence of $BiVO_4$/MWCNTs

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Abstract

Advanced oxidation processes (AOPs) have been used as analternative and effective option for treatment of waste waters especially in case of non-biodegradable compounds. It is well known that bismuth vanadate shows photocatalytic activity. The $BiVO_4$ was synthesized by sol-gel and $BiVO_4$/MWCNTs by mechanochemical method. This composite was characterized by XRD, EDX, and FESEM. The photocatalytic removal of Congo red has been studied under visible light in the presence of $BiVO_4$/MWCNTs composite. The degradation was monitored spectrophotometrically. The effect of various parameters such as pH, the concentration of dye, amount of composite, and light intensity on the rate of degradation was also studied. A suitable mechanism for the photocatalytic degradation of Congo red dye has been proposed. It is an eco-friendly method for the treatment of polluted water. It has been observed that catalyst can be recycled and used again.

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Vegetable Oil Extended High Styrene Emulsion Styrene Butadiene Rubber for Tire Tread of High-Quality Motorcycle

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Abstract

Worldwide, the quality of motorcycle has undergone revolutionary change over last decades. Technological upgradation, customer demand and road infrastructure has contributed to this revolution. These necessitate higher performance of motorcycle tires as tires being interface between powerful engines and the road. Among the various parameters of motorcycle tire tread performance, dry and wet traction, rolling resistance and mileage, are important as they conform the safety requirement, fuel economy and durability. In general, Oil-extended Styrene Butadiene Rubber (OE-SBR) with high styrene provides better traction and abrasion with little deterioration in rolling resistance properties. Here, vegetable origin oil extended high styrene (40%) SBR's were characterized in motorcycle tire tread recipe. The use of vegetable oil results in almost zero polycyclic aromatic (PCA) content and therefore, these OE-SBR's are environmentally friendly, renewable, and sustainable. SBR grades prepared with vegetable oils were showing less mixing energy, better flow behavior (low activation energy), lower filler-filler interaction (lower Payne effect) and lower tanδ@60°C as compared to petroleum oil.

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Photocatalytic properties of strontium chromate –zinc oxide nanocomposite on removal of crystal violet dye from aqueous solution

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Abstract

Photocatalysis has emerged as a promising method for degrading dyes from aqueous solutions, with diverse photocatalysts under exploration for their effectiveness. In this study, a composite of strontium chromate-zinc oxide was utilized as a photocatalyst for the degradation of crystal violet dye. The research comprehensively investigated the influence of key parameters on the reaction rate, including dye concentration, semiconductor dosage, pH of the dye solution, and light intensity. Additionally, a tentative mechanism for the photocatalytic degradation process was proposed, highlighting the involvement of superoxide anion radicals ($^{\bullet}O_2^-$) as active oxidizing species.

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A Comparative Study of the Anthelmintic Activity of *Artemisia vulgaris Linn.* and *Artemisia indica Willd.*

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Abstract

Artemisia is a annual herbaceous diverse group of plants The two plants, namely *Artemisia vulgaris* (Av) Linn and *Artemisia indica* (Ai) Willd, both belonging to Asteraceae family which comprises over 500 species distributed across temperate and cold-temperature zones worldwide. These plants are traditionally known for their vermicidal properties. The work was conducted for phytochemical screening of plant extracts and identified presence of various compounds, including alkaloids, steroids, terpenoids, and cardiac glycosides**.** The total phenolic contents were determined using the Folin-Ciocalteu method, using gallic acid as a standard**.** To assess the anthelmintic activity, earthworms (*Pheretima posthuma*) were used as a screening model. Three types of extracts from two plants were prepared petroleum ether extract, chloroform extract, and hydroalcoholic extract. These extracts were tested at different concentrations (5, 10, 15, 20, and 25 mg/ml). Piperazine citrate was used as a reference standard at concentrations (5, 10, 15, 20, and 25 mg/ml). The results of study indicated that both Av and Ai *extracts* possessed potent anthelmintic activity when compared to the reference standard, Piperazine citrate.The hydroalcoholic extracts of Artemi As a result, it can be concluded that hydroalcoholic extract of Av has higher anthelmintic activity than choloroform extract and petroleum ether extract of Av and also all three extracts of Ai, which is comparable to the standard drug Piperazine citrate. The significance of these findings suggests that the extracts from Av and Ai may have potential as natural anthelmintic agents. However, it's important to note that further research and studies are necessary to fully understand the mechanism of action and determine the efficacy, safety, and appropriate dosage of these plant extracts for use as anthelmintics in clinical settings.

Keywords*:* Phytochemical analysis, Total Phenolic Content, Anthelmintic activity, Hydroalcoholic extract.

Formulation Development and In-Vitro Evaluation of Ketoconazole Microsponge Drug Delivery System of Antifungal Drug

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Abstract

This study investigated the synthesis and characterization of Ketoconazole microsponges through the quasi-emulsion solvent diffusion method, followed by comprehensive evaluation of their properties and performance. The microsponges exhibited satisfactory production yield, loading efficiency, and particle size, with spectral analyses confirming the presence of characteristic drug peaks. Morphological assessments via SEM revealed the distinct structural differences between styrene and Eudragit microsponges. Pore characterization indicated variations in pore types and porosity between the two types of microsponges. Stability studies demonstrated no significant changes in morphology or drug release over six months of storage under accelerated conditions. Gel formulations incorporating microsponges exhibited higher viscosity and controlled drug release compared to plain drug gels. Antifungal activity assays revealed retained efficacy and potentially enhanced activity of microsponge-loaded gels compared to free drug gels and commercial formulations, along with reduced skin irritation. Overall, the findings suggest the promising potential of microsponge delivery systems for topical administration of Ketoconazole , offering controlled release, reduced irritation, and potentially improved therapeutic outcomes.

Keywords*:* Micro sponge Drug delivery system, Ketoconazole , anti-fungal activity, quasi emulsification technique.

Tree of Life: In Search of Viruses

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Abstract

The universal tree of life (ToL) has always been a topic of interest and debate for evolutionary biologists. The current tree of life follows the three domain system having bacteria, archaea, and eukarya as the major domains. Archaea and Eukarya represent sister taxons.

The placement of viruses in the Tree of Life as the fourth domain has always been a puzzle for researchers. The dilemma between the living and non-living nature of viruses has created confusion about their placement in ToL. Although several attempts have been made by scientists to construct a phylogenetic tree that includes viruses. With the discovery of giant viruses such as *Mimivirus* and the findings that they share some common genes with the other three domains gives insight into why the viruses should be included in the ToL.

Viruses complete the tree of life as they have parallelly evolved with their hosts since the beginning of life and affected the biological world. Methods such as Horizontal Gene Transfer (HGT) have enabled viruses to share their genes with other organisms and support their coevolution with their hosts. Though a perfect monocotomous branch of viruses cannot be expected due to their coevolution with the host genomes which are domain-specific, yet to depict a nearly correct representation of life, their placement is as important as any other cellular organism.

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Global Health and Infectious Diseases

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Abstract

Despite significant advances in treating infectious diseases worldwide, morbidity and mortality associated with pathogen infection remains extraordinarily high and represents a critical scientific and global health challenge. Current strategies to combat these infectious agents include a combination of vaccines, small molecule drugs, increased hygiene standards, and disease-specific interventions. While these approaches have helped to drastically reduce the incidence and number of deaths associated with infection, continued investment in current strategies and the development of novel therapeutic approaches will be required to address these global health threats. Infectious diseases today ignore geographic and political boundaries, and thus constitute a global threat that places every nation and every person at risk. Food products, livestock, exotic pets, and material goods and the microbes they carry are exchanged as cultures from every region of the world are explored. —Microbial Threats to Health, 2003

Infectious diseases continue to burden populations around the world. Both naturally occurring and intentionally introduced biological threats hold increasing potential to cause disease, disability, and death.

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Informing the Future: Critical Issues in Health: Second Edition. Biological Significance of Carotenoid Lutein and Its Role in Enhancing Vegetable Oils

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Abstract

Carotenoids and oils derived from Bharatn cultivars of Marigolds(Tagetes patula) have gained attention for their biological significance and potential health benefits. Several Bharatns suffer from nutritional deficiencies, which lead to chronic illnesses with the progression of time. Carotenoids, as antioxidants, play a crucial role in maintaining cellular health and protecting against chronic diseases. Lutein derived from Bharatn cultivars possess unique nutritional profiles and exhibit antimicrobial, skin, hair, and cardiovascular health benefits. When the carotenoid Lutein was infused into soybean oil(SBO), it improved SBO's oxidative properties significantly, thus, helping the oil retain its nutritional value when subjected to high heat. Lutein has shown excellent effects in animal studies, including preventing age-related macular degeneration, increasing cognitive function, and curbing.

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Advancement in Understanding and Combating Cervical Cancer

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Abstract

Cervical cancer remains a significant global health challenge, particularly in developing countries where access to screening and treatment may be limited. This abstract provides an overview of cervical cancer, focusing on its etiology, risk factors, screening methods, and treatment options. Cervical cancer develops in a woman's cervix. It is the 4th most common type of cancer among women, globally and 2nd most common among women in Bharat. It is mainly caused by the HPV (Human papillomavirus) . Other factor include smoking , weakened immune system , long term use of birth control pills , early sexual activity and a history of sexually transmitted infections .Treatment of cervical cancer depends on the stage and may include surgery, radiation therapy, chemotherapy or a combination. An in depth analysis of preventable nature of cervical cancer will follow, emphasizing the pivotal role of HPV vaccination in mitigating risk. Additionally, the presentation will elucidate the significance of regular screening such as pap smears and HPV testing as effective tool in combating this problem. The main matter of concern is lack of awareness, lack of availability for early stage detection and ignorance towards its symptoms. Addressing this issue through widespread vaccination, improved screening programs, global collaboration, research, treatment accessibility, prevention and increased awareness can significantly reduce the impact of cervical cancer.

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Catalyst of Change: Strategies for Tackling Global Infectious Disease Challenges

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Abstract

This paper navigates the complex web of infectious diseases elucidating their profound impact on global health. Infectious diseases are the leading contributors to mortality worldwide. From ancient plagues to modern pandemic, they have posed severe challenges to mankind. Drawing upon data from reputable global health organizations, such as the World Health Organization (WHO), National Center for Biotechnology Information (NCBI) and the Center for Disease Control and Prevention (CDC), the paper underscores the urgent need for coordinated action at the international level to address these pressing challenges.

This paper emphasizes on prevalence, mortality, morbidity, and varying transmission patterns of these diseases. Moreover, it examines the concerted efforts of global health initiatives and interventions in combating infectious diseases, showcasing vaccination campaigns, public health education programs, and access to essential healthcare services. By exploring the potential integration of traditional medicine systems like Ayurveda, one can offer holistic approaches to infectious disease management and understand the importance of cultural sensitivity in global health endeavors.

Overall, the paper serves as a comprehensive exploration of the intricate interplay between global health and infectious diseases, advocating for collective action and innovation to safeguard the well-being of populations worldwide.

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From Crisis to Resilience: Global Health Security for Pandemic Preparedness

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Abstract

In an increasingly interconnected world, safeguarding global health security is paramount to mitigating the impact of pandemics and emerging health threats. This paper delves into the critical realm of global health security and focusing on strategies imperative for effective pandemic preparedness. Beginning with an introduction to the concept of global health security, the paper elucidates its significance in "preventing, detecting and responding" to emerging infectious disease outbreaks across the borders. To bolster the credibility and solidify the findings presented herein, it incorporates data from the esteemed Global Health Security (GHS) Index. By integrating data from this authoritative source, the study underscores its commitment to providing a well-founded analysis of global health security, encompassing initiatives, challenges, and prospective solutions. Central to pandemic preparedness are multifaceted strategies aimed at early detection, establishing vigilant surveillance systems and swift response mechanisms to control the spread of infectious diseases. Additionally, it stresses the pivotal role of international collaboration, initiatives like Global Health Security Agenda (GHSA), Coalition for Epidemic Preparedness Innovations (CEPI), Access to COVID-19 Tools Accelerator (ACT-Accelerator), etc and information sharing exemplify collaborative endeavors to expedite research, equitable access, and preparedness. Drawing from lessons learned from past pandemics to the recent one, the abstract advocates for bolstering public health infrastructure, investments in healthcare systems, medical facilities, and personnel for enhancing readiness and resilience against health emergencies. Research and innovation play a critical role in advancing treatment modalities and vaccine development, underscoring the need for sustained investment in scientific endeavors. However, persistent challenges loom large. Political will, funding shortages, coordination gaps, and health inequalities pose formidable obstacles in achieving comprehensive health security. Overcoming these hurdles demands sustained commitment, strengthened surveillance systems, and concerted efforts to bridge healthcare disparities. Through collective action and unwavering determination, the vision of global health security can transcend rhetoric, becoming a tangible reality safeguarding the well-being of humanity.

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Mycobacterium tuberculosis PE_PGRS37 as a probable ATP and Calcium binding protein: a novel target for drugs that can be repurposed for Tuberculosis.

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Abstract

Mycobacterium tuberculosis (Mtb) is a fascinating and complex facultative intracellular bacterium that has impacted global health for centuries Till date, BCG is the only available vaccine against TB with low protective efficacy. Emergence of drug resistant strains made it important to have new drugs targets to be discovered. The pe and ppe gene family members which comprise approximately 8-10% of the entire Mtb genome present only in pathogenic species. (1#) PE_PGRS proteins are recently evolved members of this uncharacterized family of proteins. Proteins that are expressed at late stage of infection are important in modulating host cellular pathways. (2#) We scanned 90 days expressing proteins and found a highly disordered protein, PE_PGRS37 (Rv2126c). The presence of such intrinsically disordered regions may assist in subverting host immune mechanisms. Detailed sequence analysis of PE_PGRS37 revealed that it is an integral membrane protein with ATP (Gx2Gx5GS) and Calcium (GG-X-GX-D) binding motifs. Therefore, this protein may help the bacteria to survive in the host environment by modulating the host cellular pathways like ATP- mediated autophagy. Molecular docking of PE_PGRS37 with ATP using Pyrx gave free binding score of -5.8 kcal/mol which was comparable to already reported ATP binding protein Rv2623. (3#) Binding score of Calcium with PE_PGRS37 was found to be -1.1kcal/mol which was comparable to already reported Calcium binding protein PE_PGRS5. (4#). Furthermore, six drugs that target ATP-binding motif which are already in use against various diseases namely, crizotinib, tofacitinib, sunitinib, pyrazinamide, vemurafenib, sorafenib and regorafenib were found to bind with PE_PGRS37 with high affinity. Therefore, our in-silico data gives lead to experimentally validate the potential of PE_PGRS37 as target for drugs which can be repurposed for TB treatment.

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Quinazolines

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Abstract

Quinazolinones are interesting materials because of their valuable biological effects. In this study some new 2,3-disubstituted-4(3H)quinqzolinone derivatives were synthesized from anthranilic acid in six steps by introducing a new chiral center to the aliphatic side chain of the quinazolinone. In the last step, a single acylation on the hydrazine moiety afforded final compounds. The structures of compounds were confirmed by IR, ^{1}HNMR and Mass spectra.

Keywords: Anthranilic acid, 4(3H)-Quinazolinone, Synthesis

Assessing the Long-Term Safety profile of biologic drugs in the treatment of autoimmune diseases

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Abstract

Biologic therapies for rheumatologic diseases, which are targeted at molecules involved in the mechanisms of the immune system, provide an alternative to the existing treatment methods of disease-modifying anti-rheumatic drugs and other immunosuppressive medications. However, the current drawbacks of biologic therapies, including the inconvenience of intravenous administration, the high costs of these drugs, and the adverse events associated with them, prevent their wide use as first-line medications. This review provides an update of the recent literature on the new biologic therapies available. The review concentrates on nine drugs: tocilizumab, rituximab, ofatumumab, belimumab, epratuzumab, abatacept, golimumab, certolizumab, and sifalimumab, which are used as therapies for rheumatoid arthritis, spondyloarthritis, systemic lupus erythematosus, systemic sclerosis, or vasculitis. Biologic treatments—including five TNF-α inhibitors, the IL-1 receptor antagonist anakinra, the IL-6 receptor inhibitor tocilizumab, the selective inhibitor of T-cell co-stimulation abatacept and the B-cell-directed mAb rituximab—have provided effective therapeutic options for patients with RA with inadequate response to conventional DMARDs. However, the fact that these agents are immune modulators has raised safety concerns, prompting careful evaluation in clinical trials and intensive post-marketing surveillance. Serious infections may arise, and diagnosis may be delayed by an atypical spectrum of signs and symptoms. Patients may experience reactivation of latent tuberculosis, hepatitis B or C or opportunistic infections. RA is a risk factor for cancer, and biologic therapy may modestly increase the risk of lymphoma and some solid tumours beyond background.

Keywords: Biologics, Anti-TNF, B cell depletion, Autoimmune diseases, Rheumatoid arthritis, Spondyloarthritis, Systemic lupus erythematosus, Systemic sclerosis, Vasculitis

To Evaluate Diuretic Effect of Alcoholic Extracts of Roots of Boerhaavia Diffusa Extract (AEBD) in Rats

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Abstract

The present study was undertaken to evaluate diuretic effect of alcoholic extracts of roots of Boerhaavia diffusa extract (AEBD) in rats. The extracts were administered to experimental rats orally at doses of (2000 mg/kg) for LD50. From the LD50, doses like 1/20th, 1/10th and 1/5th were selected and considered as low, medium and high dose i.e., 100 mg/kg, 200 mg/kg, 400 mg/kg respectively. Furosemide was used as a standard drug at a dose of (10 mg/kg, p.o) in the present study. The diuretic effect was evaluated by measuring urine volume, sodium and potassium content in urine. Urine volume was significantly increased by the doses of AEBD in comparison to control group. While the excretion of sodium also increased by the test drugs. The diuretic effect of the extracts was comparable to that of standard drug. Hence the present study provides a quantitative basis for explaining use of Boerhaavia diffusa roots as a diuretic agent.

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Formulation and Evaluation of Moxiloxacin for Oral Drug Delivery System

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Abstract

The results showed that the formulation satisfied the objective of ease of administration and safety. Success of the present study recommends a detailed investigation in to in-vivo studies for its effective use in clinical practice.The alginate drug loaded micro beads well at pH 1.2 predominantly very slow but under went erosion at pH 7.2.The drug release from the micro beads was affected by the pH of the dissolution medium results more sustained effecting alkaline medium. Therefore, one can assume that Moxifloxacin hydrochloride micro beads are promising pharmaceutical dosage forms by providing sustained release drug delivery systems and avoiding the dose related side effects in the entire physiological region. The entire process is feasible in an industrial scale and demands pilot study.

Keywords*:* Moxifloxacin hydrochloride, micro beads, pH 1.2

Degradation of Brilliant Green Using Ternary Composites Involving Graphitic Carbon Nitride

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Abstract

Environmental and water pollution due to organic contaminants is a major issue all over the world. Photosensitive dyes with complex structures and long-lasting stability are highly toxic and can cause mutagenic and carcinogenic changes in humans. Heterogeneous photocatalysts using semiconductor is generally considered as an effective pathway (as green technology) for reduction of environmental pollutants via photocatalytic reaction. A ternary composites involving graphitic carbon nitride with zinc oxide and cadmium sulfide was synthesized and characterized by several techniques (Powder X-ray diffraction, Field emission scanning electron microscopy and Energy dispersive X-ray). Urea was used as precursor for the preparation of graphitic carbon nitride. The prepared composites were used as a photocatalysts for the degradation of brilliant green present in the waste water. It was found that this ternary composite can degrade brilliant green more than 80% in 90 min as evident from a decrease in absorbance. Therefore, it has been concluded that ternary composites of graphitic carbon nitride have the potential to be an efficient adaptable composite for the photodegradation of brilliant green in industrial waste water.

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Use of Z-Scheme Heterojunction of ZnO/MoS_2 For Photocatalytic Degradation of Acid Red 94

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Abstract

Dyes are commonly used in the industry for various purposes, like colouring textile, plastics, cosmetics, and even food to create vibrant and attractive products. Normally dyes are non-biodegradable and therefore, they persist in the environment. Dyes can release pollutants into water, air and soil, which can have some adverse effects on human health as well as lives of aquatic plants and animals also. Therefore, it is a demand of the day to degrade these dyes timely. Most of the chemical methods is not very much effective in degrading dyes. Here, photocatalysis enters the scene. In the present work, Acid red 94has been selected as a model pollutant and ZnO/MoS_2 as the photocatalyst. Preliminary experiments indicated that the modified photocatalyst can degrade Acid red 94successfully as evident from a decrease in absorbance of its solution. The progress of reaction was monitored spectrophotometrically at 548 nm.

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Evaluating the Pharmacological Properties and therapeutic Potential of Cannabinoids

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Abstract

There is a growing interest in the use of cannabis (and its extracts), as well as CBD oil (hemp extracts containing cannabidiol), for therapeutic purposes. While there is reason to believe that cannabinoids may be efficacious for a number of different diseases and syndromes, there exist limited objective data supporting the use of crude materials (CBD oil, cannabis extracts, and/or cannabis itself). Summary: In the present review, we examined data for pure cannabinoid compounds (dronabinol, nabilone, and CBD), as well as partially purified medicinal cannabis extracts (nabiximols), to provide guidance on the potential therapeutic uses of high-THC cannabis and CBD oil. In general, data support a role for cannabis/cannabinoids in pain, seizure disorders, appetite stimulation, muscle spasticity, and treatment of nausea/vomiting. Given the biological activities of the cannabinoids, there may be utility in treatment of central nervous system disorders (such as neurodegenerative diseases, PTSD, and addiction) or for the treatment of cancer. However, those data are much less compelling.

Keywords: cannabis extract (Δ9-THC-dominant or CBD-dominant.

Therapeutic efficacy of GSNO reductase inhibitor *for COVID-19* disease

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Abstract

Introduction: COVID-19 caused by SARS-CoV2 infection has resulted in more than one million deaths in the USA since 2019. While the vaccines against SARS-CoV2 has provided protection but infection and hospitalization continue due to evolving new SARS-CoV2 variants and unavailability of a drug targeting multi-mechanistic/muti-organ COVID-19.

Results: We studied the efficacy of GSNO Reductase inhibitors (GSNORi) in a mouse model of spike protein (SP) induced COVID-19 disease. In this study, SP1 was delivered daily via nose to C57BL/6 mice developed high fever and weight loss, **immune dysfunction manifesting as** cytokine storm (increased levels of TNFα and IL-6) in blood and lung tissue and infiltration of $CD8^+$ and $CD4^+$ T cells; (T_H1 /T_H17), macrophages and neutrophils, **ARDS associated systemic hypoxia** with increased epithelial/endothelial permeability leading to pulmonary edema and **endotheliopathy** as increased vascular CAM expression and vascular hyperpermeability, **hypercoagulability** as increased blood levels of fibrinogen, thrombin, thrombin- antithrombin complex, activated platelets, von Willebrand factor, and **brain dysfunction** as increased cerebral vascular permeability and brain edema, disease pathologies similar to human COVID-19. GSNOR inhibitor therapy protected against the multiorgan and multi-mechanistic disease pathologies described above in the SP1 mice model of COVID-19. Accordingly, GSNO or GSNOR inhibitor therapy reduced the fever and increased the body weight, decreased cytokine storm, normalized vascular permeability with decreased lung and brain edema and reduced vascular inflammation, and decreased coagulopathy markers described above

Conclusion: The observed efficacy of GSNORi (above) and it's known human safety suggest for translational potential of GSNORi for COVID-19.

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Strengthening Health Strategies with Special Reference to Persistent Organic Pollutants And The Risk Assessment Of Birth Defects

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Abstract

Persistent organic pollutants (POPs) are environmental contaminants that have been linked to adverse health effects, including birth defects. The exact mechanisms by which environmental factors affect the process of birth defects and their interaction with genetic factors remain unknown. The preventive method of birth defects especially NTD observed in both mice and humans is folic acid supplementation, but its mechanism during the embryonic process is not clear. This study aims to determine and evaluate the impact of POPs on maternal periconceptional risk of birth defects. In this study we have identified the specific POPs present in the environment that are known to cause birth defects. Additionally, we have studied the effect of POPs on periconceptional animal models to assess morphological and skeletal changes and investigated the effect of folic acid intake during pregnancy on the risk of birth defects, focusing on neural tube defects (NTDs). The morphometric observations showed significant differences between the rats pups whose mothers were exposed to pesticides. Significant decrease in the body weight of rat pups delivered was observed in pesticide exposed group i.e. chlorpyrifos (5410± 125.21 mg± SE); glyphoshate (5844±94.44 mg± SE); carbendazim (4870±65.11 mg± SE); d-trans allethrin (5643 ± 36.89 mg± SE); and Imiprothrin + cypermethrin (5514 ± 40.41 mg± SE) when compared with the control group (6243±84.11 mg± SE).In pesticides exposed group, the chlorpyrifos exposed rat pups show morphological abnormality like microcephaly, microtia, micromelia, dysmorphogenesis, distorted axis and abdominal and brain hemorrhages. Glyphoshate exposed rat pups shows abdominal and brain hemorrhages, microcephaly and micromelia abnormality. By elucidating the mechanisms by which POPs contribute to birth defects and exploring potential preventive measures such as folic acid supplementation, this study provides valuable insights into the environmental and dietary factors influencing maternal and fetal health during the periconceptional period.

Keywords **:** Persistent Organic Pollutants, birth defects, pesticides, morphometric measurements, rat neonates

Enhancement Activity of Anticancer and Cytotoxicity in Combination of Synthetic Drug and Ethanolic Extract From Ficus Religiosa (Peepal Tree) by Using Cancer Cell line Culture (Breast Cancer)

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Abstract

Herbs and Plants have been principle form of medicine in India since ancient times. Hundred of medicinal plants have been used to cure diseases. Medicinal plants played a dynamic role in manufacturing human health and improving the quality of human life for thousands of years. Medicinal plants have curative properties due to presence of various complex chemical substance of different composition. Medicinal plants have served humans well as valuable components of medicines, flavorings, beverages, cosmetics and dyes. *Ficus religiosa* is one of the medically important plants belonging to the family of Moraceae. It has been used broadly in Ayurvedic practitioner in India to treat various disease. The present work is an endeavor to compare the Invitro anticancer and cytotoxicity impact from different extracts of Ficus religiosa.

Keyword**:** *Ficus religiosa,* MTT, Ethanol Extract, Water Extract, Cell Line

Synthesize, Characterization and Pharmacological Evaluation of Isatin Derivatives.

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Abstract

Series of novel Schiff bases of Isatin the equimolar amines and 5-Dicrboxymethyl (R=COO_2Me) substituted isatins (1 mmol of each) were added to 96% w/w ethanol (20 mL) containing 8 drops of glacial acetic acid. The mixture was heated under reflux for 5 h and then cooled to room temperature. The resulting solid was collected by filtration, washed with cold ethanol and dried in open air. The derivatives thus prepared had sufficient analytical purity. anticonvulsant activity performed by method as Animals were weighed and numbered. Mice were divided into 7 groups of six animals each. Group 1 served as control which was treated with vehicle (2% v/v Tween 80), group 2 was treated with standard drug phenytoin (25 mg/kg, i.p.) and groups 3– 7 were treated with newly synthesized oxadiazole derivatives (25 mg/kg, i. p.). One hour after injection, the animals were subjected to electro shock through ear electrodes of 80 mA for 0.2 sec by electroconvulsiometer AND ANTI-inflammatory activity measured by Weigh the animals and number them. Mark the animals with picric acid for individual animal identification. Divide rats into 5 groups of 6 rats each. Note the initial paw volume of each rat by dipping just beyond tibio-tarsal junction by mercury displacement method. The pharmacological screening of the synthesized compounds showed anti convulsant activity ranging from 56.2 % to 76.3 % inhibition of epileptic seizures in mice, where as the standard drug Phenytoin showed 83.95 % inhibition of epileptic seizures in mice. The compound **iiih4** from each group was found to be nearly potent to Phenytoin which is used as standard drug. Anti-inflammatory activity ranging from 31.09 to 63.11 % inhibition of rat paw edema volume after 3 hours, whereas the standard drug Indomethacin showed 62.06 % inhibition of rat paw edema volume after 4 hours. The compound **iiih3** was found to be nearly more potent then indomethacin which is used as standard drug

Keywords: Isatin; Schiff bases; Anti convulsant activity; Anti-inflammatory activity; Isatin.

The Importance Of Generic Medicine: A Review

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Abstract

The utilisation of generic medicines plays a pivotal role in global healthcare, ensuring affordability, accessibility, and sustainability. Generic drugs, bioequivalent to their branded counterparts, offer cost-effective alternatives without compromising therapeutic efficacy. This abstract emphasises the significance of generic medicines in enhancing patient access to essential treatments, promoting healthcare cost containment, and facilitating the allocation of resources for broader health initiatives. The discussion encompasses the economic, social, and public health implications, underscoring the importance of fostering a supportive regulatory framework. This abstract also underscores the international relevance of generic medicines, emphasising their pivotal role in achieving universal health coverage and advancing global health equity.

Keywords: Generic Medicines, Affordability, Accessibility, Bioequivalence, Healthcare Sustainability, Cost-Effective

Comparative Assessment of Water Quality in Lake Pichola And Udaisagar, Udaipur

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Abstract

The quality of water in freshwater bodies is essential for maintaining ecosystem health and facilitating human activities. Lake Pichola and Udaisagar are important water features in Udaipur, Rajasthan, India, with substantial impacts on tourism, local cconomy, and cuitural legacy. Rapid urbanisation, industry, and agricultural activitics in the area may endanger the water quality of these lakes. This study work secks to evaluate and contrast the water quality characteristies of Lake Pichola and Udaisagar to determine their present condition and pinpoint possible areas for enhancing water management practices. The research utilises quantitative and qualitative methodologies such as water sampling. laboratory analysts, and socio-economic surveys. Various parameters, including pH, dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), turbidity, total dissolved solids (TDS), and nutrient levels, are assessed to analyse the physical, chemical, and biological properties of water bodics. Socio-economic surveys are undertaken to study local populations' opinions, attitudes, and bchaviours related to water consumption and conservation Initial results show disparities in water quality metrics between Lake Pichola and Udaisagar due to varying human activities, watershed features, and management strategies. Lake Pichola faces contamination from urban runofl, sewage discharge, and agricultural runoff, as well as extra pressures from tourism-related activitics and boat traffic. Udaisagar is impacted by agricultural practices and industrial activity in the surrounding region the study results will enhance the current understanding of water quality control in freshwater environments, especially in urbanised and culturally important areas such as Udaipur. Comparing Lake Pichola with Udaisagar will help evaluate existing conservation efforts and emphasise the need of coordinated management strategies to protect water quality and cosystem ealth. The project intend to provide information to policymakers, local authorities, and stakeholders to establish sustainable policies for preserving and managing freshwater resources.

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Formulation and Evaluation of Lipethosomes Containing Hydroquinone.

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Abstract

The goal of the present study was to develop niosomal gel as a nanocarrier for improved depigmentation effect of hydroquinone (HQ). As well as to evaluate the prepared niosomes for entrapment efficiency, transmission electron microscopy (TEM), zeta potential, and in vitro release study. As an ultimate point of the objectives was to evaluate the best-prepared niosomal gel formula clinically in well-diagnosed patients of melasma and the results were compared with a commercial product.

Methods: The effect of incorporation of co-surfactant such as Tween 20, Tween 40, and Tween 60 with Span 80, was studied to determine the highest entrapment efficiency and the desired release rate. Niosomes showed the highest entrapment efficiency was incorporated in different gelling agents like Carbopol 934 and Carboxymethylcellulose sodium (CMC Na) with different concentrations. Accelerated stability testing of HQ from niosomal gel formulations; the expiry date t90 was estimated. The best-prepared niosomal gel formula was studied clinically in patients of melasma and the results were compared with the commercial product (Clearique 2%)®Delta Pharma Company.

Results: There was a significant increase in the clinical efficacy of the niosomal therapy and a highly significant decrease regarding to modified melasma area and severity index (MASI), duration to achieve improvement, side effects, and the recurrence of melasma in patients treated with niosomal gel compared to the commercial product.

Conclusion: The incorporation of hydroquinone in niosomal gel improves its therapeutic effect regarding clinical effect, duration of treatment, side effects, recurrence and patient compliance.

Keywords: Hydroquinone, Niosomes, Niosomal gel, Surfactants, Co-surfactants, In vitro drug release study, Depigmentation effect

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Formulation and Evaluation of Herbal Lipstick

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Abstract

Cosmetic have become one among the daily wants of all teams in society. Every year, users are introduced to numerous new cosmetic product of the most recent trend. Cosmetics ar unimaginable in demand since historical time until day .Lipstick formulations ar most generally accustomed enhance the wonder of lips and add glamour to the touch to the makeup. With this aim and objectives, a trial was created to formulate natural lipsticks by exploitation colouring pigments of Bixa orellena linn seeds and Beta vulgaris linn root and therefore the lipsticks are evaluated for his or her organolaptic propertieslike spreading, hardness, shine and gloss and located to be satisfactory product to present engaging beauty. This eco-friendly, herbal, natural skin care product ar made up of natural plant extracts thatguarantees to rejuvenate and revitalize skin with new freshness.The practice of applying colour to cheeks and lips is very old. In ancient time, natural materials used to be applied. The preparation of this lipstick with the natural ingredients like Bixa seeds, Beet root, Olive oil, ready organic product powder of shikakai. on account of various antagonistic impacts of open manufactured readiness ,the present work was arranged by U.S.A. to define a flavoring lipsticks having minimal or no aspect impacts which can widely utilized by the women of our groups with pleasant surety and fulfillment. The present study demonstrates that both Bixa orellana and Beta vulgaris are shading specialists and Bixa orellana containing lipstick was best among both normal lipsticks.

Keywords: Herbal beauty care products, Lipsticks, Eco-accommodating

Novel Drug Approaches in Anesthesia: An Overview

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Abstract

Anesthesia is a crucial aspect of modern medicine, enabling surgeons to perform procedures and patients to undergo interventions with minimal pain and discomfort. Over the years, advancements in pharmaceutical research have led to the development of novel drug approaches in anesthesia, enhancing both safety and efficacy. This article provides an overview of some of the groundbreaking developments in this field. Anesthesiology is a medical field that focuses on taking care of patients before, during, and after surgery. In recent years, there have been significant advancements in developing new and effective methods for delivering anesthesia, which has made patient care safer, more efficient, and effective. Scientists in this field are discovering new drugs that have better pharmacokinetic and pharmacodynamic characteristics, meaning they are more efficient and have fewer side effects. Examples of these drugs include remimazolam, PF0713, and cyclopropyl methoxycarbonyl-etomidate (MOC-etomidate), which are analogues of midazolam, propofol, and etomidate, respectively. The main goal of this review is to provide an overview of these new drugs and the methods used to develop them, as well as their potential clinical applications. The review aims to give the reader an understanding of the latest advancements in anesthesia and sedation, with a focus on new drugs that are being developed and tested to improve patient care. As researchers continue to explore innovative solutions, the future holds promise for further refinements in drug formulations, delivery systems, and personalized anesthesia care. These developments are not only enhancing the practice of anesthesia but also contributing to the overall advancement of surgical and medical procedures.

Keywords: local anesthetic; general anesthetic, Clinical anaesthesia, etomidate, midazolam, propofol, Remimazolam, Dexmedetomidine, AZD-3043 (TD4756), JM-1232 (-) (MR04A3),

A Study on Clincal and Laboratory Profile of Scrub Typhus Patients Diagnosed at A Tertiary Care Hospital From Southern Rajasthan

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Abstract

Background: Scrub typhus is fast growing, potentially fatal and most neglected rickettsial disease emerging in India mostly responsible for Acute Undifferentiated Febrile Illness(AUFI) in patients.

Material & Methods: A total of 981 serum samples of patients with suspected scrub typhus were received in Microbiology lab from April 2023 to December 2023. Scrub typhus was tested by ELISA. All detailed clinical history, physical examination, reports of standard set of investigation was obtained from the case file.

Result: 84 samples were reactive by ELISA test. Among these patients, fever (100%) was the most common symptom. The most predominant sign noted in our study was icterus in 38% cases followed by hepatosplenomegaly(14%). Elevated transaminase level was detected in 65% cases followed by increased serum urea/creatinine level and thrombocytopenia in 47% and 35% cases respectively.

Discussion: Fever was the most common symptom reported in all 84 (100%) patients, similar finding was also reported by Sudhir K Verma et al and Rajendra Prasad Takhar et al. A study conducted by Verma et al and Kedareshwar P.S et al [16] both reported icterus as the most predominant sign in 28.8% and 53.3% cases respectively, where as a study conducted by Raman Sharma et al most common clinical sign was hepatosplenomegaly reported in 50.4% patients. A study conducted by Lakshmi RMMV et al in which elevated transaminase and increased serum creatinine level was noted in 82.7% and 20.6% respectively, which is similar to our present study.

Conclusion: Hence we conclude that scrub typhus is an important differential diagnosis in patients with fever, thrombocytopenia, icterus, elevated serum transaminase and patients with acute hepatitis and multiorgan dysfunction. High index of suspicion in patients with AUFI and prompt treatment can significantly reduce complications thereby decreasing both morbidity and mortality.

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Use Of Green Composite for Photocatalytic Degradation of Methyl Violet

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Abstract

A green composite has been utilized for photocatalytical degradation of Methyl violet. The effect of different parameters have studied like Amount of catalyst, initial concentration of Methyl violet and initial pH medium .Methyl violet concentration was determined by UV-Vis spectrophotometry. The green composite is a Mixture of plant leaves with nanoparticle of Metal and graphene oxide FTIR, X-ray powder diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDAX)were used to characterize the synthesized nanocomposites. Purposed study involves use of bio-absorbent (Eco-friendly and low cost) and also involves waste treatment of unused plant dried parts. It's easy handle biowaste worldwide. The result of the elemental analysis indicated that this green composite in leaf having a elemental composition of oxygen (33.75%) iron (29.43%) magnesium (8.67 %) aluminium (8.17%) carbon (5.00 %) copper (8.20%) and sulfur (1.45%) .

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Evaluation of Antimicrobials Activity of Selected Indigenous Medicinal Plants

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Abstract

Herbal medicine refers to the use of any plant's seeds, berries, roots, leaves, bark, or flowers for medicinal purposes. Along with other dosage forms, herbal drugs are also formulated in the form of ointment. An ointment is a viscous semisolid preparation used topically on a variety of body surfaces. The objective of the study was to evaluate the Pharmacognostical, Phytochemical and evaluation of the antimicrobial herbal ointment from the different extracts of dried leaves of selected medicinal plants like Aerva Lanata, Bauhinia variegata, Acmella uliginosa. The anti-Microbial properties of extracts were evaluated by Agar well diffusion method using gram positive bacteria like Staphylococus aureus, Bacillus subtilius, gram negative bacteria like Escherichia coli, Klebseilia pneumonia. Amongst the test extracts, the results suggested that, Methonolic extracts showed significant anti-Microbial activity compared with standard drug. Plants show high efficiency of antimicrobial activity due to the presence of various phytochemicals, antimicrobial tests of the combinations were carried out. The most effective combination was then determined by comparing the results of the zone of inhibition. Then the minimum inhibitory concentration of the effective combination was found out.

***Keywords*:** Poly Herbal ointment, antimicrobial activity, minimum inhibitory concentration, irritancy, spreadability, diffusion, stability

Synthesis, Characterization and Antibacterial Activity of Newer Drugs of Sulfamethoxazole Derivatives.

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Abstract

The synthesis of the considered compounds has been successfully achieved. 2. Characterization & identification of the target compounds were confirmed by determination of the physical properties, FT-IR spectroscopy ,1H-NMR spectra and elemental microanalysis. 3. Our study of the biological activity indicated that Compounds (M3-8) can be further explored as antibiotic agents.

Keywords: FT-IR spectroscopy ,1H-NMR spectra, elemental microanalysis.

Studies on Polyurethane coating based on Modified Castor oil, Commercial acrylate polyols and Polysiloxane

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Abstract

The polycondensation reaction of commercial acrylate polyols (AP), 2,4-Tolylene diisocyanate (TDI) and modified castor oil (MCO) [Castor oil-succinic anhydride-pena erythritol reaction product] at various proportions was carried out and afforded polyurethanes (PUs). To neutralize end –NCO groups, these PUs reacted with monocarbinol terminated polydimethyl siloxane (MTPS). The resultant PU coatings were applied on MS steel panels at room temperature. All the PU coatings were characterized by physical, chemical and mechanical properties.

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Hydrotropic Solubilisation Of Nimuslide For Parental Administration

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Abstract

Nimesulide is a non-steroidal anti-inflammatory drug (NSAID) that exhibits analgesic, antipyretic and anti-inflammatory activities. It is practically insoluble in water. The effect of various hydrotropes such as nicotinamide, sodium ascorbate, sodium benzoate, sodium salicylate and piperazine on the solubility of nimesulide was investigated. The solubility enhancement of nimesulide by the hydrotropes was observed in decreasing order as piperazine > sodium ascorbate > sodium salicylate > sodium benzoate > nicotinamide. In order to elucidate the probable mechanism of solubilization, various solution properties of hydrotropes such as viscosity, specific gravity, surface tension, refractive index, specific conductance of hydrotropic solutions were studied at 25 +/- 2 degrees C on the basis of earlier studies. The hydrotropic solubilization of nimesulide at lower hydrotrope concentration may be attributed to weak ionic interactions while that at higher hydrotrope concentration may be due to molecular aggregation. Parenteral formulations using piperazine as a hydrotrope were developed and studied for physical and chemical stability.

Keywords: nimesulide, hydrotrope concentration, piperazine as a hydrotrope.

Formulation and Evaluation of Organic Poly-Herbal Hair Oil

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Abstract

Humankind uses various products known as cosmetics to enhance elegance, to look young and charming. Thus, cosmetics play a keen role in human life. Cosmetology is defined as the science of alteration in appearance. Herbal cosmetics have burgeoning demand and in the world market and are inestimable gift of nature. There are wide spans of herbal cosmetic products to satisfy beauty regime and have less side effects when compared with synthetic drugs. Hair plays a very important role in enhancing the personality of humans as well as it acts as a protective appendage. The presence of number of phytochemical and natural constituents in the organic poly-herbal hair oil have dual work, one that the formulation is used as a cosmetic for hair-care and the other that the presence of phytochemical amend the hair care and protection, which naturally results in healthy hair. The present work is aimed to develop effective organic poly-herbal hair oil for daily use and to prevent various hair problems, including alopecia and scalp psoriasis. Four formulations were prepared using different types of oils, along with various herbs/parts of herb. These oils were subjected to evaluations for organoleptic properties, chemical and analytical basis. All four formulations were compared based on the result of evaluations and the effective one was selected as the best.

Keywords: cosmetics, phytochemical, hair-care, organic poly-herbal hair oil.

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Role of Nutraceutical in Management of Chronic Diseases

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Abstract

Nutraceuticals have received considerable interest because of their presumed safety and potential nutritional and therapeutic effects". The concept of nutraceuticals was stared from the survey in U.K., Germany and France which concluded that diet is rated more highly by consumers than exercise or hereditary factors for achieving good health. In recent years there is a growing interest in nutraceuticals which provide health benefits and are alternative to modern medicine. By using nutraceuticals, it may be possible to reduce or eliminate the need for conventional medications, reducing the chances of any adverse effect. Nutraceuticals often possess unique chemical actions that are unavailable in pharmaceuticals. The entire world is fighting diseases characteristic of the modern age such as obesity, osteoporosis, cancer, diabetes, allergies, and dental problems. With a global increase in the prevalence of obesity, both nutrition and exercise play key roles in its prevention and treatment. Nutrients, herbals and dietary supplements are major constituents of nutraceuticals which make them instrumental in maintaining health, act against various disease conditions and thus promote the quality of life. Using food products to promote health and cure disease is renowned. Currently most of the drug molecules available in the formulations were anciently used in their crude form.

Keywords*:* Nutrient, Disease (osteoporosis, cancer, diabetes, allergies, and dental problems) and treatments,Future food, Medicine.

Simultaneous Determination of Genotoxic Impurities and process impurities in Amlodipine Besylate by reverse phase High performance liquid chromatography

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Abstract

A Simple accurate precise cost effective Gradient HPLC method was developed and validated for quantification of 4 process impurities. (2-Chloro Benzyl Mono chloride,1-Chloro-2-DichloroMethyl Benzene, Amlodipine Besylate Imp-1 and Imp-2.). Both Chloro impurities are GTIs alert and hence covered at TTC level of 117ppm and remaining two impurities are covered at 0.10%. Common method developed for GTIs and ICH level impurities. The method was developed on HPLC with mobile phase sodium, phosphate buffer and pH adjusted to 3.5 with orthophosphoric acid. Gradient method developed with buffer and acetonitrile. Fused core new technology was adopted for method development so that run time of HPLC method will be Less. Acescentis express ES CN with 15cm x 4.6mm, 2.7micron column was used. Dual Wavelength was selected for GTIS and nor ICH impurities. (220nm and 280nm). Flow rate was 1.2ml/min and injection volume were 5 microlitre. The was validated as per ICH guidelines, All the parameter of ICH covered during method validation, Specificity, system suitability, LOD, LOQ, Linearity, Precision, and Accuracy. Based on validation data this can be used in routine quality control for release of commercial batches.

The benefit of the method is QC release the using one single of GTIS and ICH level impurities. No need to go for two different. Here the cost and time of batch release reduce to 2-fold.

Keywords: Drugs Impurity, HPLC Method Validation, Amlodipine besylate

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Synthesis, Chemistry and Biological Activity of Some Novel Thiazole Derivatives

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Abstract

This present work deals with the synthesis, characterization and anti-inflammatory activity of some novel thiazole derivatives. 2-amino thiazole (I) was prepared by triturating thiourea and iodine and mixed with substituted acetophenone. Equal mole of (I) & Chloroacetyl Chloride in the presence of potassium hydroxide, at room temperature afforded (II). The chemical structures of synthesized compounds were confirmed by MASS, FTIR and ^{1}H-NMR spectral studies. The synthesized compounds were (50µgm/kg) screened for anti-hypertensive activity by Tail Cuff method.

Keywords: Anti-hypertensive activity, Tail Cuff method, Thiazole, Thiadiazole.

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Formulation and Evaluation of Enteric Coated Tablet of Rabeprazole Sodium

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Abstract

The prepared powder blend was evaluated for pre compression parameters like angle of repose, bulk density, tapped density, compressibility index and Hausner ratio. The obtained results indicated that it has good flow property.

Rabeprazole Sodium enteric coated tablets were prepared by wet granulation method. The prepared tablets were evaluated for hardness, thickness, weight variation, friability, assay and disintegration time. All these parameters were found to be within the pharmacopoeial limits in F-V formulation.

Rabeprazole Sodium enteric coated tablets were coated with Cellulose acetate phthalate and Diethyl phthalate in different concentrations.

In vitro dissolution study was carried out for F-V formulation showing better drug release than the marketed product. The drug release was found to be 99.12 % at 60 minute

The accelerated stability studies of F-V formulation at 40 ºC/75 % RH for a time period of 3 months indicated that there was no significant change in description, disintegration time, drug content and in vitro dissolution profiles. The result shows that the F-V formulation was stable for 3 months.

From all the above observations the study concluded that the enteric coated tablets of Rabeprazole sodium (F-V) formulation was better one compared to the other formulations.

Keywords: Rabeprazole sodium, Diethyl phthalate, Hausner ratio.

Formulation And Evaluation of Liposomes Containing Tretinoin

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Abstract

Partition coefficient is calculated by the ratio of equilibrium concentration of a dissolved substance in a two phase system they are octanol and water. The partition coefficient of Tretinoin was found out to be 6.29. Solution was scanned under UV-Vis Spectrophotometer and λ max was determined. It was found to be as per the monograph. All dilutions and measurements were made in methanol and the absorbance was taken at λ_{max} 340 nm against a reagent blank. The standard curve was plotted between absorbance and concentration. A number of clinical studies have now demonstrated the superiority of liposomal drug formulations over conventional delivery systems. In this respect, liposomal formulations have been successful in treatment of a number of dermatological diseases and disorders such as psoriasis, mycoses, idiopathic hirsutism and cutaneous infections.

Keywords: psoriasis, mycoses, idiopathic hirsutism, cutaneous infections.

Investigating the Impact of Pharmacist-led Interventions on Medication Adherence and Patient Outcomes.

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Abstract

The aim of this study was to provide a scoping review of the impact of pharmacist-led interventions on medication adherence and clinical outcomes in patients with hypertension and hyperlipidemia. A scoping review was conducted using pre-defined search terms in three scientific databases, including Google Scholar, ScienceDirect, and PubMed. A multi-stage screening process that considered relevancy, publication year (2009–2019), English language, and article type (original research) was followed. Review articles, meta-analysis studies, and conference proceedings were excluded. Data charting was done in an iterative process using a study-specific extraction form. Of the initially identified 681 studies, 17 studies with 136,026 patients were included in the review. Of these, 16 were randomized controlled trials, while the remaining study was a retrospective cohort study. The majority of pharmacist-led interventions were face-to-face counseling sessions (n=8), followed by remote- or telephone-based interventions (n=5) and multi-faceted interventions (n=4). The majority of the studies (n=7) used self-reported adherence measures and pharmacy refill records (n=8) to measure the rate of adherence to prescribed medications. Eleven of the included studies reported a statistically significant ($P<0.05$) impact on medication adherence. Overall, twelve studies assessed the effect of the interventions on the clinical outcome measures; of these, only four studies were associated with significant impact.Pharmacist-led interventions were associated with improved patients' adherence to their medications but were less likely to be consistently associated with the attainment of clinical outcomes. Face-to-face counseling was the most commonly used intervention; while, the multi-faceted interventions were more likely to be effective in improving the overall outcome measures. The rigorous design of targeted interventions with more frequent follow-ups, careful consideration of the involved medications, and patients' characteristics could increase the effectiveness of these interventions.

Keywords: adherence, hyperlipidemia, antihypertensive, pharmacists, intervention, pharmacy services

Green Synthesis of Silver Nanoparticles

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Abstract

The appearance of nanotechnology significantly changed the drug sciences and incredibly improved the diagnostics and treatment of different illnesses that compromise human existence. A few metallic nanoparticles are widely utilized as nanomedicines because of their likely restorative applications. Among them, silver nanoparticles are noteworthy because of their exceptional synthetic and actual properties. This survey talks about sorts of nanoparticles, and green blend techniques alongside their decrease instruments, including financially reasonable lessening materials like green growth, kelp and blossoms. Aside from climate amicable strategies, a few organic exercises, for example, wound recuperating, antibacterial, antifungal, hostile to growth, against viral, and so on, are portrayed exhaustively. Subsequently, we have zeroed in on how silver nanoparticles upgrade designated drug conveyance and the component of medication discharge alongside their poisonous impacts.

Particles with a size scope of 1-100 nm are considered nanoparticles (NPs), and silver nanoparticles (AgNPs) have been profoundly successful antimicrobial specialists. The huge surface area of AgNPs is the essential consider that results better antimicrobial movement because of solid collaboration with miniature life forms even at a lower focus. As AgNPs discharge silver particles inside microorganisms to kill them, numerous systems have been proposed making sense of the activities of AgNPs on microbes, for example, obstructing the respiratory chain, protein denaturation because of solid clinging to practical gatherings, impeding vehicle of supplements to the bacterial cell layer, streaming out cell contents by upsetting the phone film and hindering deoxyribonucleic corrosive (DNA) replication. Thus, AgNPs go about as an intense dispensing with specialist against microscopic organisms, including Gram-negative and Gram-positive. AgNPs have been synthesized by physical, chemical, photochemical, microemulsion, biological and microwave methods.

This strategy has diminished the utilization of perilous synthetic substances to combine the AgNPs. The utilizations of AgNPs are more extensive than those of different NPs as they have shown massive and dynamic jobs in the clinical field, exhibiting against parasitic, hostile to bacterial, hostile to diabetic, hostile to disease impacts, and so on. Magnificent natural movement with low poisonousness to solid cells and critical harmfulness to disease cells has been accomplished by plant-based AgNPs.

Keywords: Silver Nanoparticles, green synthesis

Telemedicine and Digital Tools in the Treatment of Major Depressive Disorder (MDD)

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Abstract

MDD is a serious and life-altering condition that can lead to significant functional impairment and is associated with considerable economic burden, morbidity and mortality. Researchers and clinicians are address the growing global health and economic burden of major depressive disorder (MDD) during the COVID-19 pandemic, likely due to lockdowns. The recognition and treatment of MDD presents a challenge that may not necessarily be overcome with a single treatment course or therapy. Treatment of MDD often involves psychotherapy, pharmacotherapy or a combination of both. Apart from traditional way of treatment, new paths are introduced like telemedicine and digital tools. The use of telemedicine for mental health treatment increased significantly during the COVID-19 pandemic. Digital psychotherapy, including person-to-person telemedicine visits or text-message exchanges with a therapist, has been demonstrated to be an effective way to deliver high-quality therapy to patients, especially those in remote settings. Given that digital psychotherapy has effectiveness comparable to that of in-person visits and has utility in reaching patients in both rural and urban areas, its use has been incorporated into clinical practice guidelines in several countries. Benefits of digital psychotherapy may include greater accessibility, convenience and cost-effectiveness, which reduce the likelihood of lost appointments, thus promoting continuation of care. Present presentations focused on the digital tool treatment landscape for MDD is evolving to incorporate multiple modes of therapy that aim to improve care and access to care for patients.

Keywords: Major Depressive Disorder, Telemedicine, Digital Psychotherapy

Effect of Herbal Medicine "*diabetocure*" on Clinical and Biochemical Parameters of Metabolic Syndrome.

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Abstract

Around 400 herbal treatments for diabetes mellitus are reported, but only a few of these have been approved of their therapeutic efficacy. Traditional treatments have mostly disappeared in occidental societies, but some are prescribed by practitioners of alternative medicine or taken by patients as supplements to conventional therapy. A hypoglycemic action from some treatments has been confirmed in animal models and non-insulin dependent diabetic patients, and various hypoglycemic compounds have been identified. The herbal substitutes for insulin and related anti-diabetic drugs seems challenging, but herbal treatments can provide valuable clues for the development of new oral hypoglycemic agents and simple dietary adjuncts.

***Keywords**:* Diabetes, Insulin, Metabolic, Hypoglycaemia, Alloxan

Evaluation of Immunomodulatory and Anticancer Activity of Plant Derived Chemicals

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Abstract

Psoriasis – autoimmune disease is a chronic T-cell mediated disease which affects 125 million people worldwide and the management of psoriasis is a daily challenge for dermatologists as diverse morphological changes which can worsen the disease, can be seen in patients with this disease. Since the disease is chronic inflammatory in nature, risk of developing skin cancer in patients with psoriasis is high. Literature states that there are no known methods which lead to permanent control of this disease and natural derived drugs have a good efficacy and potential in controlling the symptoms of psoriasis without side effects thus promising the successful treatment strategies.

Objective: To evaluate the ethanolic extracts of selected two medicinal plants – CM and CO and combination (CM+CO) for *in-vivo* immunomodulatory model to cause a total effect of combination extract higher than the sum of single effect of each extract.

Methodology: The extracts of selected plants (leaf part) were prepared by using maceration technique using ethanol as a solvent. Acute oral toxicity study was performed as per the OECD guideline 423. The anti-psoriatic activity of extracts was assessed using imiquimod induced psoriasis in mice based on acute oral toxicity tests.

Results: The LD50 value of ethanolic extract of CM and CO were found to be in category 5 i.e. >2000 – 5000 mg/kg, with LD50 cut off at 5000 mg/kg body weight. For Imiquimod induced psoriasis in mice model, significant results were reported for parameters like body weight, ear thickness and spleen weight as compared to disease control group. Significant reports were reported in estimation of cytokines TNF-α and IL-6.

Conclusion: The extracts were found to be effective in treating psoriasis in mice model and has shown effects on cellular immune responses (T cells) and proven its therapeutic potential.

Keywords: Psoriasis, skin cancer, plant extracts, imiquimod, mice model, LD50,

Formulation and Evaluation of 100% Herbal Hair Dye

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Abstract

The word herbal is a symbol of safety in contrast to the synthetic one which has adverse effects on human health. Herbal preparations viz., herbal tablets, herbal tonics, herbal paste, herbal shampoo, herbal contraceptives and herbal dyes has become popular among the consumer herbal medicines represent the fastest growing segment to heal the various ailments. A dye can generally be described as a colored substance that has an affinity to the fiber, fur or hair. Melanin is what gives color to human skin, eyes, and hair. It's the ratio of two types of melanin Eumelanin and Pheomelanin that determines your natural hair color. Hair dyes include dyes modifiers, antioxidants, alkalizers, soaps, ammonia, wetting agents, fragrance, and a variety of other chemicals used in small amounts that impart special qualities to hair such as softening the texture or give a desired action to the dye. The chemicals that are normally used in the dye are amino compounds (4-amino-2-hydroxytoluene and m-Aminophenol). Metal oxides, such as titanium dioxide and iron oxide, are also often used as colorants in the process. Continuous usage of such compounds containing dye on natural hair causes so many side effects such as skin irritation, erythrema, loss or damage of hair and skin cancer. The main aim and objective of present study is Formulation and evaluation of Herbal Hair Dye, investigating the alternative to the synthetic and semi synthetic dyes.

Keywords: Melanin, Eumelanin, Pheomelanin

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Synthesis, Characterization and Antimicrobial Evaluation of Novel Quinoline Derivatives

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Abstract

This present work deals with the synthesis, characterization and biological screening of some novel quinoline derivatives. 2-(quinolin-8-yloxy) acetohydrazide III was synthesized according to a known method. The key intermediates, 2-(quinolin-8-yloxy) acetohydrazone derivatives IIIa-e were synthesized by the condensation of 8-quinolinoxyacetic acid hydrazide with different aromatic ketones. The chemical structures of synthesized compounds were confirmed by MASS, IR and H-NMR spectral studies. The synthesized compounds were (25, 50, and100 µg per ml) screened for anti microbial activity by paper disc diffusion method.

Keywords: Quinoline, biological screening, aromatic ketones, paper disc diffusion method.

Harnessing Nanotechnology: Advancements in Controlled Drug Delivery using Chitosan modified PLGA (Poly(lactic-co-glycolic acid)) nanoparticles

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Abstract

Chitosan modified PLGA nanoparticles have evolved as promising approach for improving the performance and efficacy of PLGA NPs drug delivery, renowned for their biocompatibility and biodegradability. Despite their efficacy, PLGA NPs face certain limitations such as cholinesterase degradation ,rapid drug release etc. By integrating chitosan, known for its mucoadhesive properties and pH-responsive behavior, onto PLGA NPs, Chitosan modified PLGA nanoparticles have been shown enhancing drug delivery by mitigating burst release issues. Using a high-gravity rotating packed bed (RPB) method, chitosan-PLGA NPs were synthesized and loaded with paclitaxel (PTX) as a model drug. Results demonstrated improved drug loading, encapsulation efficiency, and sustained drug release profiles compared to unmodified PLGA NPs. Additionally, chitosan modification facilitated increased cellular uptake of the nanoparticles, leading to enhanced cytotoxicity against cancer cells, sustained drug release and enhanced drug toxicity, suggesting that chitosan-modified NPs can be used as carriers of anticancer drugs. Overall, chitosan-modified PLGA NPs present a promising platform for achieving controlled drug release and enhancing the therapeutic efficacy of drugs.

Keywords: chitosan; PLGA nanoparticles; controlled drug delivery release; nanotechnology;

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A Comprehensive Review of Influenza Virus and its Comparative Account with other Respiratory Viruses

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Abstract

Influenza virus belonging to the family *Orthomyxoviridae* remains to be a perennial concern of public health resulting in yearly epidemics and pandemics occasionally. The virus can be divided into four types namely A, B, C and D out of which influenza A and B are known to affect humans. According to WHO, influenza is responsible for nearly 500,000 respiratory deaths every year. Transmission occurs via droplets from an infected person and symptoms include fever, cough, myalgia and even pneumonia in severe cases, often complicated by bacterial co-infections. The novel pandemic strains are mainly genetically reassorted influenza A viruses that can cause high morbidity among the immunologically naive population. Diagnosis is commonly done by polymerase chain reaction (PCR) tests.

Prevention can be done by vaccination however the available antiviral treatments have to be regularly revised owing to the high evolution rates of influenza virus. The emergence of strains with genetic variations can be attributed to the phenomena of antigenic drift and shift. Metagenomic studies and phylogenetic analysis are necessary tools for tracing the evolutionary history of the influenza virus genome in order to identify the conserved regions which can be useful targets for the formulation of antiviral drugs and vaccines to combat the widespread influenza virus.

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CRISPR/Cas9 as an Antidote for Cancer Therapy

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Abstract

CRISPR/cas9 has become a powerful innovation of a decade and has simplified changes in the genetic properties of an organism. The CRISPR/cas9 has been derived from auto-defense mechanism observed in prokaryotes. It contains a target specific single guide RNA and cas9 endonuclease. A target specific sgRNA transmits cas9 protein to a target site. Due to this, it lays a promising future towards finding a suitable and effective cancer research. This paper will also contain the multifunctional nature of CRISPR-Cas9 which is an advanced tool in cellular processes, including cell proliferation and immune responses with gene therapy for glioblastoma. Further scope of both has been laid out and lastly, analysis of pros and cons of CRISPR technology has been displayed along with systematic pathway. Future scope has been discussed.

Keywords: CRISPR/cas9, cancer, immune therapy, gene therapy, glioblastoma

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Cobalt Oxide-Graphitic Carbon Nitride Nanocomposite As Efficient Photocatalyst For Degradation Of Azure B Dye

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Abstract

A simple one step pyrolysis method was used for synthesis of Cobalt oxide-graphitic carbon nitride nanocomposite for the present study. The precursor used here for graphitic carbon nitride is abundantly available urea. The synthesised samples were characterised by X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM) and Energy dispersive X-ray (EDX). The presence of cobalt oxide was confirmed by EDX. The flower like morphology observed in FESEM. The XRD confirmed the crystalline nature of the nanocomposite. The photocatalytic degradation of Azure B was observed under visible light using synthesized nanocomposite as photocatalyst. The various parameters like pH, concentration of dye, amount of composite and intensity of light was also observed. The present investigation showed the increased photocatalytic activity of nanocomposite as compared to g-C3N4 and cobalt oxide alone.

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Photocatalytic Reduction Of Sodium Carbonate To Formaldehyde Using Graphitic Carbon Nitride – CdS – $BiVO_4$ Composite

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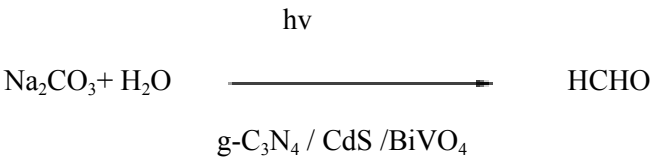
Abstract

Growing energy demand challenges and environmental problems due to fossil fuel consumption have raised awareness in recent decades. Currently, the world's energy needs are largely dependent on fossil fuels such as oil, coal and natural gas. World energy consumption is constantly increasing over time with social living standards and industrialization. To solve both of the most pressing problems; the photocatalytic reduction of carbon dioxide to produce synthetic fuels can be an attractive solution to limit environmental pollution. The conversion of CO_2 into value-added chemicals by visible light driven photocatalysis has a great potential. A small amount of the composite was added to the solution of sodium carbonate soluble form of carbon dioxide in alkali and then the solution was exposed to visible light to reduce it to formaldehyde. The progress of the reaction was monitored spectrophotometrically using chromotropic acid. The effect of different operating parameters on the formation of formaldehyde was evaluated.

Keywords: Photocatalysts, Graphitic carbon nitride ($g\text{-}C_3N_4$), Environment sustainability heterojunction, Climate changes, Global warming, Sodium carbonate, Formaldehyde.

Graphical Abstract –



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Analysing Isothermal and Kinetic Aspects of Nickel Adsorption onto Activated Carbon Derived from Bio Diesel Waste

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Abstract

This study aimed to tackle the issue of excessive Nickel (Ni) pollution in industrial effluents, surpassing the recommended threshold of 0.006 mg/ml. By utilizing biodiesel waste, specifically Jatropha husk waste, to produce Activated Jatropha Husk Carbon (AJHC), the research focused on efficiently removing Ni to achieve water quality suitable for recycling. Factors such as contact time, temperature, pH, initial Ni concentration, and activated carbon dosage were investigated for their impact on Ni adsorption efficiency. Optimal results were achieved at pH 6 (77.7%), an initial Ni concentration of 10 mg/lit (83.9%), an adsorption dose of 0.5 gms/lit (59.4%), a temperature of 60°C (80%), and a contact time of 4 hours (73.2%). The Freundlich isotherm model and pseudo-second-order kinetic model were well-fitted for the adsorption process. The study concluded that biodiesel waste is a valuable raw material for cost-effective and environmentally friendly Ni removal from wastewater using AJHC.

Keywords: Biodiesel waste, Ni removal, adsorption efficiency, adsorption kinetics, adsorption isotherm.

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Photocatalytic Degradation of Congo Red Over $FeWO_4$-CuS Particulate System

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Abstract

The photocatalytic degradation of Congo red has been studied under visible light in the presence of $FeWO_4$ – CuS composite as a photocatalyst. Ferric tungstate was prepared by hydrothermal method. The photocatalytic activity of $FeWO_4$ - CuS composite was evaluated for photodegradation of Congo red dye under visible light. As-prepared composite was characterized by techniques such as XRD, EDX and FESEM. The effect of various parameters was investigated on rate of degradation and optimum conditions were obtained as pH = 9.0, concentration of Congo red = 1.20 x 10^{-4} M, amount of $FeWO_4$ – CuS = 0.10 g and light intensity = 70.0 mWcm^{-2}. It was observed that composite has the highest catalytic activity in basic medium. A tentative mechanism for the reaction has been proposed involving hydroxyl radical as an active oxidizing species.

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Photocatalytic Degradation of Indigo Carmine Dye with the Help of Composites of Nickel Vanadate Titanium Dioxide

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Abstract

Photo catalysts are an uncommon tool for sensibly and environmentally friendly Disposal of large ordinary particles like insecticides and dyes. Here, we can make use of a Variety of techniques for evaluating wastewater treatment. It is a good way to eliminate Contaminants from wastewater and transfer them into a water cycle with astoundingly good Environment protection. The most well-known photogenic substance is TiO_2. A few different Types of recognised light-responsive image feasible catalysts have been examined by Numerous experimenters. Here, TiO_2 , Nickel vanadium oxide and its composites can be Used. We can degrade Indigo caramine dye with the help of and nickel vanadium oxide and TiO_2 composite.

Keywords: Indigo caramine dye, doubly distilled Water, nickel vanadium oxide, and titanium dioxide.

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E-waste and It's Management

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Abstract

Electronic waste (e-waste) poses environmental challenges due to hazardous components. Green chemistry offers sustainable solutions for e-waste management, involving eco-friendly processes to recover valuable materials. This includes techniques like solvent-free extraction, bioleaching, and recycling methods that minimize environmental impact and promote a circular economy.

Green chemistry techniques with its 12 principle:

Prevention: Design processes to prevent waste.
Atom Economy: Maximize the incorporation of all materials used.
Less Hazardous Synthesis: Choose safer materials and methods.
Designing Safer Chemicals: Develop chemicals with reduced toxicity. Safer Solvents and Auxiliaries: Minimize the use of auxiliary substances. Design for Energy Efficiency: Optimize energy usage during synthesis. Use of Renewable Feedstocks: Prefer renewable raw materials.
Reduce Derivatives: Minimize the need for protective groups or derivatization. Catalysis: Use catalytic reactions to increase efficiency.
Design for Degradation: Ensure products break down into innocuous substances. Real-time Analysis for Pollution Prevention: Monitor and control processes to avoid waste.

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Synthesis of Drugs by Reduction Process

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Abstract

The synthesis of the drug requires the reduction of a nitro group (47), which was identified as a bottleneck in its synthesis. Nitro-reduction in halogen-substituted aromatic rings is generally challenging due to competitive side reactions such as debenzylation and dehalogenation.

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Synthesis of Products by Oxidation Process

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Abstract

Oxidation is the second most common degradation pathway for pharmaceutical after hydrolysis. Oxidation is mechanistically more complex and produces wider range of degradation products.

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Application of Hot Melt Extrusion in the Development of a Stable High-Energy Amorphous Solid Dispersion of a Poorly Water-Soluble Drug

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Abstract

Formulation of active pharmaceutical ingredients (API) in high-energy amorphous forms is a strategy to enhance solubility, dissolution rate and, consequently, oral bioavailability of poorly water-soluble drugs. Hot Melt Extrusion (HME) technology is currently being used in the pharmaceutical industry due to several advantages over traditional processing methods to prepare solid dispersions. A class IV drug with low solubility and bioavailability, a folate antimetabolite
(FM), widely used in the treatment of malignancies was selected for the studies. Melt extrudates of the drug and polymer (Kollidon VA 64) were prepared at various proportions using ThermoScientific Haake Minilab twin screw extruder at 20%, 30% and 40% drug loads and temperatures of 175-180 °C. Span 20 was used as a solubiliser at 8 % levels to the various drug
loaded extrusions. Melt extrudates with various drug loads and their formulations (with Avicel and poloxmer added externally) were stored in amber glass bottles at 25 °C/60% RH open and 40 °C/75% RH open for 1 to 12 months. The DSC and dissolution studies were carried out for the extrudates. The amorphous melt extrudates with 30% drug load prepared using KVA 64 showed higher solubility and dissolution properties and was physically and chemically stable at controlled room temperature for at least one year, and the prognosis for longer-term stability was good.

Keywords: Hot Melt extrusion, solubility, solid dispersion, dissolution, stability

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CRISPR/CAS9 Applications: A Potential Tool for Targeted Genome Editing

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Abstract

CRISPR/Cas9 is an effective gene editing aid with multiple applications for the treatment of numerous diseases and protection from numerous diseases. It is adapted from an immune system of bacteria. Clustered regularly interspaced short palindromic repeat (CRISPR) and their associated protein (Cas-9) is most efficient and accurate method of genome editing aid in all living cells and utilized in many application. CRISPR/Cas9 has been engineered into a genetic editing tool applicable in any organism, becoming without doubt a revolutionary tool in genome editing, enabling researchers to precisely manipulate specific genomic elements, and facilitating the function elucidation of target genes in biology and diseases. This review will be mainly focused on the wide expansion of CRISPR technology in agriculture, through inducing desired alterations in plants, and the fascinating aspect of it in medicine thorough improving immunotherapy, especially antiretroviral therapy by finding the cure for HIV. Due to the higher efficiency of CRISPR/Cas9 compared to other editing approaches, it has been widely investigated to treat numerous hereditary and acquired illnesses, including cancers, hemolytic diseases, immunodeficiency disorders, cardiovascular diseases, neurodegenerative conditions, and a few X-linked disorders. CRISPR/Cas9 system has been used to treat cancers through a variety of approaches, with stable gene editing techniques.

Keywords: CRISPR, Cas-9, Genome editing, Target Genes, Agriculture, Immunotherapy, Antiretroviral, Cancers, Immunodeficiency, Neurodegenerative, X-linked disorders.

AI-Powered Translational Medicine: Integrating Chemistry, Biology, and Artificial Intelligence for Enhanced Healthcare Solutions

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Abstract

The integration of artificial intelligence (AI) with chemistry, biology, and translational medicine represents a pivotal advancement in healthcare. This convergence signifies a transformative force poised to revolutionize scientific research, medical diagnosis, treatment strategies, and patient care. Leveraging the complementary strengths of diverse disciplines, AI-driven integrative methodologies offer unprecedented opportunities to tackle intricate biological challenges and translate fundamental discoveries into tangible improvements in health outcomes. This review paper embarks on a comprehensive exploration of the profound impact of AI-enabled integration on healthcare enhancement. Through an exhaustive review of pertinent literature, case studies, and emerging trends, the paper elucidates the transformative potential of AI-driven integration in driving medical breakthroughs and shaping the trajectory of personalized medicine. Drawing from sources indexed in databases such as PubMed/Medline, Scopus, and EMBASE, the present study delves into the effects of implementing AI in healthcare environments and anticipates outcomes stemming from its deployment. Incorporating AI into healthcare holds tremendous promise in enhancing disease diagnosis, treatment selection, and clinical laboratory testing. By harnessing vast datasets, AI tools surpass human capabilities by discerning intricate patterns across various healthcare domains, offering heightened precision, cost efficiency, and time-saving benefits while mitigating the likelihood of human errors. At the crux of this integration lies the synergy between AI, chemistry, biology, and translational medicine. AI algorithms demonstrate remarkable capabilities in analyzing vast amounts of biological data, identifying patterns, and predicting outcomes with unprecedented accuracy. In the context of chemistry, AI-driven approaches facilitate the design of novel molecules, streamlining the drug discovery process and expanding the repertoire of potential therapeutics. In biology, AI-powered analytics aid in the interpretation of genomic, proteomic, and metabolomic data, guiding the development of targeted interventions. Translational medicine serves as the conduit between basic scientific research and clinical practice, aiming to translate laboratory findings into tangible benefits for patients. By integrating AI with chemistry and biology, translational medicine can accelerate the pace of innovation and improve patient outcomes. AI-enabled diagnostics aid in the early detection of diseases, leading to timely interventions and improved prognosis.

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Synthesis of Novel Indolotriazine Derivatives and Evaluation of their Biological Activities

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Abstract

The indole nucleus exhibits extensive spectrum of biological activities such as anticancer, anti-tubercular, antioxidant, antimicrobial, antidepressant, antiepileptic etc. The main objective of this study was to design, synthesize novel derivatives of indolo triazines, and its substituted nucleus using various aromatic aldehydes to afford title compounds 3-(2-(-2-substituted benzylidene cyclohexylidene) hydrazinyl)-5H-[1,2,4] triazino [5,6-b]indol-8-amine (MC1-15) followed by screening for its biological potency. 5-fluoroisatin was treated with thiosemicarbazide to form 8-fluoro-5H-[1,2,4]triazino[5,6-b]indole-3-thiol (1) which on treatment with hydrazine hydrate yields (8-fluoro-5H-[1,2,4]triazino[5,6-b]indol-3-yl)hydrazine(2).The comp 2 treated with cyclohexanone to give (8-fluoro-5H-[1,2,4] triazino[5,6-b]indol-3-yl))cyclo hexylidenehydrazine (3). A mixture of 3a treated with substituted benzaldehyde in the presence of alkali forms (8-fluoro-5H-[1,2,4]triazino[5,6-b]indol-3-yl))-2-substituted benzylidene cyclohexylidene) hydrazine. MC1-15 recrystallized from absolute ethanol. The synthesized compounds were characterized by IR, ^{1}H-NMR and mass spectral data and screened for their in vitro antioxidant property **by** using DPPH, NO and H_2O_2 methods. The screening was done for four concentrations of the synthesized compounds (25, 50, 75, 100 µg/mL). Most of the compounds had shown good antioxidant activity against ascorbic acid.

The presence of electron donating substituent on indole ring enhances the activity. Antibiotics fight against bacterial infections but the commonly used antibiotics have become less effective due to emergence of drug-resistant bacteria hence, it is essential to investigate newer drugs with less resistance. This study was carried out with an objective to investigate the antibacterial and antifungal potentials of the synthesized compounds using paper disc diffusion method.

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Repurposing the Dark Genome – I: Antisense Proteins

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Abstract

Based on the expression patterns, genomes are divided into three categories: sequences that encode proteins, sequences that encode RNA, and sequences that don't participate in expression processes. Recent sequencing and annotation have confirmed that a minor portion of the genome is tasked with protein encoding, while a significant section encodes RNA, and the remaining portion of DNA sequences does not actively contribute to the expression of genes. This allocation ratio varies among different organisms. Is it feasible to create proteins and peptides synthetically using non-expressive sequences? This study extends the prior research conducted by Dhar et al. in 2009 (i), which involved creating intergenic proteins in E. coli. It explores the possibilities of making functional genes and proteins from antisense DNA sequences (ii). We computationally translated antisense strands of 4315 protein-coding genes in *E. coli* and 6317 genes in *S. cerevisiae*, producing 32 and 10 full-length proteins, respectively. Among these, 9 in *E. coli* and 7 in *S. cerevisiae* were found to be unique. Furthermore, antisense proteins exhibited isoelectric points, instability indexes, and hydropathy values in the promising range, suggesting potential structural stability if these proteins were expressed within cells. Many of the antisense proteins indicated strong possibilities of transporter and enzyme functions. Currently the experimental validation studies are going on. Designing novel antisense genes, RNA, and proteins/peptides from the dark genome points to a huge untapped space that may yield a wealth of information from cell physiology, evolutionary, and application perspectives.

Key Words: Antisense protein, non-expressing, protein-coding.

References:

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Review on the Recent Development of Tacrine Hybrids as Potential Candidates Against Alzheimer's Disease (AD)

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Abstract

Nitrogen-based heterocyclic compounds are essential for medicinal chemistry and the pharmaceutical industry. The basic nitrogen atoms can be incorporated both as amino substituents and as part of a ring itself. Replacing just one carbon atom of a carbocyclic ring with a heteroatom changes the physical as well as chemical properties of the resulting molecule. The electron-rich Nitrogen functional group readily accepts or donates a proton, and also quickly establishes diverse weak interactions. N-heterocycles bind with a variety of enzymes and receptors in biological targets with high affinity due to their improved solubility.[1] Nearly 75% of unique small-molecule drugs contain a nitrogen heterocycle. As a result, the N-heterocyclic compound is selected over other heterocyclic compounds for the drug design.[2] N-heterocyclic compound Tacrine is the first FDA-approved drug for the symptomatic treatment of progressive neurodegenerative disease i.e., Alzheimer's disease (AD). In 1998, tacrine was discontinued due to its significant side effects, particularly hepatotoxicity.[3] However, tacrine has been selected as the ideal active fragment because of its simple structure, low molecular weight, clear activity, easy crossroads into BBB, and superiority in structural modifications. This review covers recent efforts in the synthesis and biological screening of tacrine-based compounds from 2021-2024.

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Microbiological analysis and Quality aspects of Drinking Water

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Abstract

Water is essential to life but many people do not access clean and safe drinking water and many die of waterborn disease.most of the countries in world are suffering from water born disease and this adversely affecting our environment and human health. Contamination in water is mainly caused by Microbes .Microbes are single celled organisms that are invisible to the naked eyes. They could only be seen under microscope , they make up almost 60 % of the earths living matter. Micro organisms can survive in any type of environment .

Aquatic ecosystem are very important to maintain high level of biodiversity, livelihood and productivity of biosphere. The presence of antimicrobial (antibiotics), antimicrobial resistant bacteria and antimicrobial resistant gene in aquatic environment is cause of concern for human health because aquatic environment is a main key transmitter route for spreading of disease. AMR (Antimicrobial Resistance) occur when pathogen no longer respond to medicine or antimicrobial agents and when antibiotics agents become ineffective, than infection become impossible to treat.Some of the common microorganisms that affect our drinking water and cause harm are : Balantidium coli , Entamoeba histolytica , Giardia lamblia , Escherichia coli. Some of the diseases caused by microorganisms which are harmful are Amoebic dysentery , gastroenteritis ,cholera , typhoid , jaundice , diarrhoea , skin disease. Some of the obvious cause of micro organism in water : Improper treated sewage , runoff from animal waste ,septic system ,human faecal matter ,fertilisers, pesticides and other chemicals that have been applied to land near water. We can analysis drinking water quality that it is contaminated or not by physical test like colour , turbidity [suspended solids] ,odour and taste and also by chemical test like pH [(pH should be 6.5 to 8.5) and B.O.D.

Keywords **:** Microbes, contamination, drinking water, typhoid , Escherichia coli , sewage treatment

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Remediation of Polluted Environment by the Use of Nanoparticles Derived from Metallic Trash

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Abstract

To sustain life and to carry out a number of industrial processes, water is an absolute must. In industrial wastes, dyes are a big environmental problem because they stay in the environment for a long time[1]. Textile, paper, and leather industries frequently utilize these dyes because of their bright colours, but they are resistant to degradation, which can lead to water contamination[2]. When dyes are introduced into water bodies, they can cause disturbances in aquatic ecosystems, affecting both plant and animal life. Moreover, certain dyes may encompass hazardous substances, thereby presenting potential dangers to both human well-being and biodiversity[3]. For the sake of preserving water quality and ensuring the sustainability of industrial activities, it is essential to address the disposal of dye-contaminated wastewater from industrial processes.

This study followed the concepts of the circular economy by utilizing metallic waste generated from diverse industrial operations to synthesize nanoadsorbents. We performed an electrochemical procedure to generate nanoadsorbents. The produced nanoadsorbents underwent characterization utilizing several techniques, including Fourier transform infrared (FTIR) spectroscopy, Powder X-ray diffraction (PXRD), Scanning electron microscopy (SEM), Elemental dispersive X-ray (EDX), Transmission electron microscopy (TEM) etc. The results indicate that the synthesized nanoadsorbents possess an average crystallite size of 16.29 nm and predominantly exhibit a spherical form. UV-visible spectroscopy is also employed to confirm the adsorption of azo dye. The findings indicate that the developed nanoadsorbent possesses the capacity to adsorb the dye and effectively purify the polluted wastewater. Its adsorption efficacy is 98% in just 10 seconds, which is really astounding.

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Efficient Access of β-amino Cyclohexanone via Titanium (IV) Isopropoxide Catalysed Amine Conjugate Addition to Enone (ACAE)

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Abstract

Presence of β-aminocarbonyl compounds are widely distributed in pharmaceutical agents and natural products including alkaloids and polyketides. This structural core is also integral part of several biologically important molecules which serve as powerful anti-biotic and drug molecules.[1,2] *Lewis acid catalysed amine conjugate addition to the electron deficient α,β-unsaturated ketone* is the most efficient strategy to synthesise β-aminocarbonyl compounds.[3] However, reported methods suffers from several limitations such as poor substrate scope, harsh reaction conditions and scalability. Most importantly most of these methods are limited to the acylic ketones.

As part of our ongoing research program directed towards the development of new conjugate addition reactions[4], our primary goal is to solve this issue. Here in we report the first titanium(IV) isopropoxide catalysed *Amine Conjugate Addition to the Enone* (ACAE) at room temperature. This methods works well for both electron-deficient as well as electron-rich functional groups and total 32 β-aminocarbonyl compounds have been synthesised utilising this methods.[5] This method is scalable up to gram scale and enantioselective amine conjugate reaction is under investigation.

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Deep Eutectic Solvent as Greener Alternative for Dissolution Enhancement of Drugs

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Abstract

Over 40% of newly developed chemical entities (NCEs) in the pharmaceutical industry face significant challenges due to their practical insolubility in water, resulting in slow drug absorption and variable bioavailability [1]. This fundamental challenge emphasizes the crucial requirement for techniques aimed at enhancing solubility in drug development. However, many traditional organic solvents utilized in solubility enhancement processes pose environmental and health risks [2]. For that reason deep eutectic solvents (DES) have emerged as promising green alternatives for improving solubility and bioavailability [3]. Furthermore, DES exhibit potential applications in pharmaceuticals, including enhancing permeation and stability of active pharmaceutical ingredients (APIs) and facilitating the development of more effective formulations [4, 5, and 6]. Their customizable properties make DES a superior choice compared to conventional solvents. This review emphasizes the potential of DES as a valuable technique for enhancing the solubility and bioavailability of BCS class 2 drugs."

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Guardians of the Mosquito Realm: How Pacifastin Influence the Malaria Parasite and its Vector?

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Abstract

As per the WHO World Malaria Report 2023, 249 million malaria cases were estimated globally in 2022, out of which India accounts for 3.389 million cases. The two major vectors of *Plasmodium sp.* in India are *Anopheles stephensi* and *Anopheles culicifacies*. Within biological systems, proteases are a class of molecules that are both abundant and pervasive, serving as both regulators and catalysts. Serine protease is one such essential enzyme that both the organisms (*Anopheles* and *Plasmodium*) are endowed with. These enzymes are crucial for the survival of pathogens and vectors. The inhibitors targeting these enzymes create the possibility as therapeutic targets.

Endogenous serine protease inhibitors are found in almost all classes of arthropods as a negative feedback mechanism for enzymatic reactions. The prophenoloxidase pathway in insects which is catalysed by the serine proteases (trypsin and chymotrypsin) is negatively regulated by Pacifastin (an endogenous serine protease inhibitor). Likewise, the genome of *P. falciparum* contains several serine proteases that are members of the subtilisin, chymotrypsin, and rhomboid protease clans, and they temporally control expression in both the asexual and sexual phases of the parasite life cycle.

This study focuses on the characterisation and mechanism of action of Pacifastin with respect to parasite and its vector. We have found the refolded recombinant Pacifastin (rPac) to be functionally active via enzyme inhibition study. Dot-blot confirmed the interaction of rPac with chymotrypsin. Additionally, when recombinant Pacifastin was exogenously subjected to the third instar larvae of the *Anopheles stephensi,* it delayed the metamorphosis phenomenon. Since chymotrypsin is a highly conserved protein among living organisms therefore, our hypothesis that the *Anopheles stephensi's* rPac could lower the parasitaemia *in vitro* by inhibiting its serine proteases. Our future goal is to decipher its function by siRNA knockdown study in *P. vivax* and *P. falciparum* infected *An. stephensi* adult females.

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Chemoenzymatic Route to Synthesize Bicyclic Nucleoside analogues

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Abstract

Nucleosides are one of the most widely studied compounds. Nucleoside analogues have been a point of interest for chemists and biochemists due to their role in nucleic acid biosynthesis and various other biologically significant processes such as viral replication and division of cells[1]. In the past few decades, a variety of artificial or modified nucleosides have been synthesized by chemists to incorporate them in the antisense oligonucleotides or to screen their biological activities such as antiviral, anti-HIV, anticancer, antimetabolites, antisense properties, and many more [2]. We have developed a convergent route for the synthesis of a new class of bicyclic nucleoside. The synthetic route to the corresponding arabino-configured uracil and thymine bicyclic nucleosides proceeds in 24 and 27% overall yields, respectively, starting from 1,2,5,6-di-O-isopropylidene-α-D-glucofuranose. This synthetic protocol includes some crucial steps such as Vorbrüggen base coupling and chemo-enzymatic regioselective acetylation of the primary hydroxyl group by using Lipozyme® TL IM where it was found that Lipozyme® TL IM could be recovered and reused for selective acetylation without losing its selectivity.

Key words: Nucleosides, regioselective, base coupling

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Characterization of Zeolite-Y Encapsulated Zn(II)Salmphen Complex with Targeted Anticancer Property

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Abstract

Resistance and severe side effects of classical chemotherapeutic drugs are the major challenges to cancer therapy[1]. New therapeutic agents and combination therapy are considered as a potential solution that enhances the efficacy of the drug as well as reduces drug resistance[2]. The success of a platinum-based anti-cancer drug, cisplatin has paved the way to explore metal-centered anticancer therapeutic agents. A wide range of transition metal complexes have been investigated for anticancer activity, and some of these complexes even outperform cisplatin. However, majority of these complexes lack tumor cell selectivity and are extremely lethal to noncancerous cells[3]. Numerous Salen and Salophen based metal complexes have been explored for their biological activity, but Salmphen metal complexes have not been attempted. This report[4] describes the synthesis and characterization of Zn(II)Salmphen and zeolite-Y-encapsulated Zn(II)Salmphen complex using elemental analysis, FTIR, UV–Vis, Fluorescence, PXRD, FESEM, and XPS techniques. The encapsulated Zn(II)Salmphen complex exhibits fluorescence in DMSO, DMF, DCM, and chloroform with an additional feature compared to its neat analogue. The cytotoxicity of both free-state and zeolite-Y encapsulated complex is examined against cancer (MCF7) and noncancerous (HaCaT) cells. Our results demonstrate that in comparison to cisplatin, encapsulated Zn(II)Salmphen complex have better activity against cancer cells and most importantly, it is less toxic to noncancerous cells. Overall, zeolite encapsulated Zn(II)Salmphen complex could be a better alternative to traditional drug cisplatin with minimal effect on noncancerous cells and can also be utilized as a fluorescent probe in exploring the mechanistic pathway of its activity against cancer cells.

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Repurposing the Dark Genome – II: Reverse Proteins

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Abstract

In the genome's blueprint, three distinct sequence categories emerge: sequences accountable for protein encoding, RNA encoding, and sequences that play no role in expression. We asked: If evolution favoured sequences for metabolic functions, to what extent is untapped (non-expressing) and underutilized (solely RNA encoding) information accessible for continued innovation? These questions drive us to experimentally create functional proteins through the utilization of intergenic sequences from E. coli, as published by Dhar et al. in 2009 [i]. This ongoing study extends the scope of the original report and explores the potential of reading naturally evolved genes in reverse order to unlock novel proteins or peptides. Using the full length reverse gene data in *C.elegans*, we computationally translated 20,000 *C. elegans* protein-coding genes in reverse direction to construct a virtual library of 188 'full-length and first-in-the-class' proteins [ii]. Here, we present a brief account of these reverse proteins in terms of their sequence similarities, structural details, stability, function and cellular address. This approach opens up new opportunities of designing novel proteins and peptides towards functional outcomes. Currently the experimental studies are going on. In future, we plan to expand the search space to other model organisms and provide a public access of this new data for further experimental validation.

Keywords: Reverse coding, synthetic proteins, synthetic biology, genomics.

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Functional Expansion and Diversification of HSP40s in Human Malaria Parasite

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Abstract

Human malaria parasite has evolved an efficient protein folding machinery to keep their metastable or aggregation prone proteome in functional state (1,2). A unique feature of human malaria parasite, *Plasmodium falciparum* is the specific expansion and diversification of HSP40 family that serve as co-chaperones of HSP70 in different cellular compartments (3,4). Many of them have diverged from human orthologs and also show sequence variation within *Plasmodium* species. Herein, we have explored the functional diversity of cytosolic, organellar and exported HSP40s. Our biochemical studies suggested that cytosolic and apicoplast HSP40 suppresses aggregation more efficiently than nuclear and exported HSP40. Whereas, the exported HSP40 effectively binds and protects unfolded substrates in comparison to cytosolic and organellar HSP40s. Limited proteolysis experiment gave insights into the differences in their conformational dynamics and stability. Using peptide-spot arrays containing *Plasmodium*-specific peptides with different physiochemical properties, we characterized the client recognition motif of different HSP40s. Apicoplast-resident HSP40 had specifically higher binding to hydrophobic and neutral peptides, whereas, cytosolic HSP40 binds to hydrophilic peptides. BLI experiments done with control peptides gave insights into their binding kinetics (association and dissociation constants). Ultracentrifugation assays with parasite lysate showed that these HSP40s formed higher-order complexes with their co-chaperones and substrates. Experiments are ongoing to check their cellular expression and localization under different proteotoxic stress conditions and identify their probable interacting partners. These studies will open avenues to understand parasite biology and identify alternative sites of intervention.

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To Evaluate the Effectiveness of Curry Leaves on Worm Infestation Among Children

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Abstract

Worm infestations contribute significantly to global burden of disease in children especially in tropical and subtropical regions. Intestinal nematode infestation with round worm, hook worm, whip worm and tape worm are the source of severe morbidity condition in children as well as in adult represented by about five hundred to thousand million people globally. The distribution of these diseases caused by these infestations extends throughout the communities of poor and socio economically deprived people in the countries of tropics and subtropics. Curry leaves is one of the most commonly available herbs in the tropical area and have immense potentialities in treatment of worm infestation and other diseases. The daily intake of curry leaves powder will prevent the worm infestation in the children as well as in adult that will enhance the health of the children.

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Exploring molecular mechanism of genital rotation in Indian Anopheles Mosquito

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Abstract

Anopheles culicifacies and Anopheles stephensi are two major malaria vectors in India. Controlling vectors is a very effective strategy of controlling malaria, however mosquito population eradication is extremely challenging as they develop resistance against all classes of insecticides very rapidly. Apart from insecticide treatment, one of most successful strategy of mosquito (Aedes) control is Wolbachia (bacterial) treatment which generally develops sterile male mosquito. However, this strategy is not very effective in Anopheles mosquito.

Currently, our knowledge about male Anopheles mosquito maturity or its role in reproduction is very limited. Recently it was documented that the rotation of genital part of male mosquito is required for sexual maturity, however underlying physiological and molecular events that lead to sexual maturity of male anopheles' mosquito is completely unexplored. In this work we have studied male mosquito maturity under different conditions (for e.g., temp, food, insecticide exposure) and determined how different factors influening mosquito maturity. In addition, we have also performed detail transcriptomic analysis of different stages of mosquito in order to identify set of genes responsible for male mosquito maturity. We believe this information will enrich our current knowledge about reproductive biology of male anopheles' mosquito. Furthermore, this study can also provide valuable insight about male mosquito sterility which has big implication in malaria control.

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Synthesis of Thiourea Based Biologically Active Potent Inhibitors of Hepatitis B Virus

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Abstract

Hepatitis B Virus is a hepatotropic virus that may cause acute and chronic liver infection in humans. Currently, 3.5 percent of the total world population is chronically infected with HBV that are managed using a combination of antiviral and immune modulatory therapies. A candidate molecule 1-(3-(1H-imidazol-1-yl)propyl)-3-(2,4-difluorophenyl)thiourea (coded as IR-415) exhibiting excellent antiviral efficacy in cell culture model was identified after a high-throughput screening of the Maybridge library. We undertook the synthesis of twenty derivatives of IR-415 and evaluated them for their in vitro activity against hepatitis B virus. It was observed that on changing the linker carbon between the phenyl thoiurea and imidazole ring of the parent compound from three carbon propyl to four carbon n-butyl there was a significant improvement in anti-hepatitis B viral activity. The human hepatoma HepG2 cells transfected with HBV genomic DNA or HBV-permanent cells (HepG2.2.15) were treated with different concentrations of synthesized 20 IR-415 derivatives. Inhibition in the expression of viral proteins (HBsAg, HBeAg, HBx etc.) was observed significantly in two antiviral candidate drug outoff 20 derivatives compared to IR415. The in vitro results corresponded with the in-silico studies performed on these two selected thiourea derivatives with HBx protein.

***Keywords**:* Hepatitis B, thiourea, antiviral, HBx protein

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Evaluation of Thyroid Dysfunction in Coronary Artery Disease Patients

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OBJECTIVE: - To estimate the status of Thyroid Function Test (TFT) in a coronary artery disease (CAD) patient.

BACKGROUND:-Thyroid hormones are very vital for the normal functioning of heart. Cardiovascular manifestations are frequent findings in both hypothyroidism and hyperthyroidism. Both hypothyroidism and hyperthyroidism can produce changes incardiac contractility, myocardial oxygen consumption, cardiac output, blood pressure and systemic vascular resistance. [1] In hyperthyroidism, there is a link between low serum concentrations of T3 and T4 and a reduction in cardiac output, heart rate, stroke volume and myocardial contractility **(Toft and Boon, 2000)[2].** The guidelines for heart failure produced by the American College of Cardiology and the American Heart Association support conducting thyroid function tests in patients with heart failure to determine if thyroid dysfunction is a primary contributor to heart failure. [3]

MATERIAL AND METHODS: - The study is a cross-sectional study, which was carried out in Pacific hospital, Udaipur, Rajasthan in the Department of Biochemistry**.** Subjects between 25-60 years of age group, who have diagnosed with overt or Subclinical hyperthyroidism / hypothyroidism according to Thyroid profile Test (TFT) and 100 cases of thyroid dysfunction is undertaken to study the cardiac manifestations by lipid profile. The subject was both male and female.

RESULT: - In the present study. In Hyperthyroid Patients, Females (56.2%) were more than males (43.7%) in this study. This female preponderance in hyperthyroidism is well known. In this study commonest cardiovascular symptom was found to be Palpitation (69.6%), followed by Dyspnoea (30.4%) and Chest Pain (4.3%). Palpitation and Dyspnoea are the common symptoms of Hyperthyroidism. In this study 82.4% patients had overt hyperthyroidism compared to 17.6% patients, who had subclinical hyperthyroidism. In Hypothyroidism majority patients were in the age group 20-40 years. Females were more than males. Among cardiovascular symptoms breathlessness was the commonest symptom, followed by palpitation, chest pain.

CONCLUSION: - We concluded that, in Hypothyroidism Patient, the Majority patients were in the age group 20-40 years. Females were more than males. Among cardiovascular symptoms breathlessness was the commonest symptom, followed by palpitation and chest pain. In Hyperthyroidism patient, the Majority of patients were in the age group 41-60 years. This study is to reveal the association with risk factors such as age and dyslipidaemia, which play a significant role in the progression of Thyroid dysfunction.

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Decoding the Mechanism of Refractoriness : Genomic and Proteomic analysis of *Anopheles culicifacies* Subspecies

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Abstract

Malaria, a prevalent health concern, and mainly transmitted by Anopheles mosquitoes. In India, *Anopheles stephensi* and *Anopheles culicifacies* serve as primary vectors in urban and rural areas, respectively. Notably, *Anopheles culicifacies* is a major contributor to malaria transmission in the country, consisting of five sibling species designated as A, B, C, D, and E. Among these, A and E have the disease transmission capability, whereas B subspecies demonstrates complete refractoriness to disease transmission. Identification of these subspecies has been facilitated through the utilization of the Mitochondrial COII gene, with a full length of 684bp observed for all anopheline taxa except *Anopheles culicifacies*, where it is 530bp.

Our preliminary data revealed the distinct nucleotide variations between subspecies A, D, and subspecies B, C, and E. Despite existing reports on the identification of B subspecies, a comprehensive characterization is notably absent in the literature. This study aims to rectify the gap by employing a molecular and proteomic approaches to identify and characterize the B subspecies. The outcome of this research is to forecast and enhance our understanding of the molecular mechanisms underpinning the refractoriness of the B subspecies, thereby contributing to the reduction of malaria burden.

Dedicated to our beloved Late Prof. Ashok K. Prasad

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Efficient One-Pot Synthesis and Photophysical Characterization of Base-Modified Fluorescent Nucleosides

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Abstract

Base-modified fluorescent nucleosides are of great interest due to their high sensitivity towards the micro-environment and are utilized as powerful tools for investigating nucleic acid structure and functions. [1,2] 5-substituted-2′-deoxyuridines had been studied due to their potent activity against different viruses. These nucleoside monomers have also exhibited high anti-leishmanial and anti-bacterial activities. [3,4]

We have synthesized a series of highly fluorescent novel 5-(3″-alkyl/aryl-Amino-1″-azaindolizin-2″-yl)-2′-deoxyuridines by the atom economical Multi-component Groebke–Blackburn–Bienayame (GBB) reaction following two different strategies. In strategy A, diacetylated 5-formyldeoxyuridine was reacted with a variety of 2-aminopyridines and alkyl/aryl isocyanides under optimized GBB reaction conditions followed by deacetylation of the resulting GBB products to afford 5-azaindolizino-2′-Deoxyuridines in 83 to 95% overall yields. In strategy B, diacetylated 5-formyldeoxyuridine was first deacetylated, which on GBB reaction under standardized conditions with 2-aminopyridines and alkyl/aryl isocyanides afforded the desired 5-azaindolizino-2′-deoxyuridines in 21 to 23% overall yields, which clearly indicates that strategy A is far more efficient than strategy B. All the synthesized compounds were found to be fluorescent and exhibited significantly higher absorption and emission bands (Stokes shift in the range of 59–126 nm) compared to their precursor nucleoside, thymidine, due to the large extended conjugation. Thus, they potential molecules for the study of local structure and dynamics of nucleic acids involving them. Moreover, the synthesized highly fluorescent nucleoside derivatives are suitable for the synthesis of modified oligo-nucleotides involving them, which can be used for hybridization with the complementary DNA strand to study the local geography of DNA.

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Renal Impairment in Industrial Workers Occupational Exposed to Textile Dye in Pali District

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Abstract

Background: The workers from textile processing and dyeing industry are exposed to various processing chemicals, dyes and different pollutant for long term which may causing hazardous effects on various organs like particularly kidney, liver have become important issue. Renal impairment among workers exposed to organic solvents as nephrotoxic substance or in the worst case scenario the development of end- stage kidney failure.

Objective of study: To evaluate the Renal Function test in Textile Factory workers.
Materials and Methods: Present study was conducted on 100 Case group (exposed occupationally) and 100 Control group (non exposed occupationally) of either sex. Renal function test was analyzed using fully automated Biochemistry Analyzer Beckman Coulter AU480. Result were subjected to suitable statistical analysis using student 't' test and p-value.
Result: serum creatinine and blood urea level is more in Textile processing and dyeing industry workers than non-exposed occupationally.
Conclusion: serum urea, serum creatinine, was significantly increased in the textile processing and dyeing industry workers ($P < 0.001$) as compared to that of controls ($P= 0.000$). High serum levels of creatinine, and blood urea considered to be indicators for the damaging of the tubular epithelium. Nephrotoxicity caused by organic solvents is reversible once the exposure has increased awareness and early diagnosis of the exposure to toxic substances in textile processing and dyeing industries are essential for performing prompt management, improving clinical outcomes

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Serological Responses Against Plasmodium Vivax Circumsporozoite Protein (Pvcsp) From Three Geographically Diverse Malaria Endemic Regions Of India

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It is an important step for designing a malaria vaccine, identifying highly immunogenic antigen which can be immunogenic in different eco-epidemiological areas. The *Plasmodium vivax* sporozoite surface protein circumsporozoite protein (PvCSP), whose role in sprozoite development, motility and cell invasion, has made it the leading pre erythrocytic malaria vaccine candidate. PvCSP is a ~36 kDa protein which contains N-terminal, a central repeat region and a highly conserved C-terminal. Central repeat region has 9 amino acid long 19 repeats, which are highly immunogenic. In this study recombinant PvCSP was expressed as a soluble form, of a molecular mass ~31 kDa, by E. coli expression system and specifically recognized by monoclonal antibody and P. vivax patient sera. A total of ~300 blood samples will be collected from individuals living in three different eco-epidemiological settings Nadiad, Ranchi and Chennai in India. Indirect ELISA was performed to measure human IgG antibodies against recombinant PvCSP antigen. The difference in seroprevalence and factors associated with antibody responses at each site was statistically analysed. The data shows significant natural acquired antibody response against the recombinant PvCSP. Results of this study will give an insight of immune status of people living in these three settings and also support the malaria vaccine development program.

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Industrial Waste Water Purification Using Iron Oxide Nanoparticles Synthesised From Recycled Materials

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Azo dyes are synthetic colourants that are widely utilised in textile, printing, and cosmetics industries. They are known for their bright colours and ease of use, but they can release poisonous aromatic amines that can harm the environment and human health[1-2]. Unfortunately, the production and use of Congo red and other azo dyes have raised environmental concerns due to their major contribution as a water pollutant. Congo red pollution is largely caused by the discharge of wastewater from factories that utilise this dye[3]. Efforts are being made to regulate their use, develop safer alternatives, and promote sustainable practices to minimize their environmental impact.

In this investigation, we used a circular economy approach by recycling metal scrap from industry as a component in creating nanoparticles. For producing iron oxide NPs, we used electrochemical method with scrapped rusted iron nails as electrodes. In this technique, we used 50mM ferrous sulphate solution as an electrolyte and a direct current power supply. Different methods were used to characterise the synthesised iron oxide NPs, including ultraviolet-visible (UV-visible) spectroscopy, Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), and transmission electron microscopy (TEM). The results demonstrated that the synthesised iron oxide NPs have an average crystallite size of 7.54 nm. Iron oxide NPs has potential to adsorb Congo red dye hence prepared NPs have been utilised for the adsorption of Congo red dye.

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Exploring cuticular proteins and their role in insecticide resistance development in malaria vector *Anopheles stephensi*

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Abstract

Introduction: Vector control through the use of chemical insecticides has played a pivotal role in the worldwide decline of malaria cases. Insecticides penetrate through mosquito cuticle and variation in cuticular composition and thickness may result into slow insecticide uptake resulting in insecticide resistance development. Cuticle comprises several cuticular proteins (CPs) belonging to different sub-group protein families in cuticle. There is a lack of data on cuticular proteins in Indian malarial vector, *An. stephensi.*

Aim: To investigate the altered genotypic expression of cuticular proteins among laboratory reared insecticide susceptible and resistant *Anopheles stephensi*.

Methodology: Insecticide susceptibility bioassays were conducted to determine the resistance status of *An. stephensi* against deltamethrin as per standard WHO protocol. Total RNA was extracted using the Trizol method for both resistant and susceptible mosquitoes followed by cDNA preparation using Takara first strand synthesis Kit. The quality of the cDNA was measured by the PCR amplification of actin specific primers for the *An. stephensi* mosquitoes. Expression of cuticular genes CPR127 and CPR63 was determined using gene-specific primers. Amplified products were visualised on a gel. Genotypic expression was quantified using Takara Sybr green for the qRT-PCR.

Results: Genotypic expression analysis reveals alteration in the expression levels of CPR127 and CPR63 genes among insecticide resistant versus susceptible female *Anopheles stephensi* mosquitoes. Both CPR127 and CPR63 genes were upregulated with ~3.3 and ~2.5 log fold change respectively among resistant female *An. stephensi* as compared to susceptible mosquitoes.

Conclusion: Understanding the differences in the expression of the cuticular proteins in the cuticle of resistant and susceptible mosquitoes will highlight their role in the development of insecticide resistance by malaria vectors.

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Therapeutic Potential of Artemisinin-Coated Iron Oxide Nanoparticles for Targeted Hyperthermia in Gastric Cancer

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Abstract

Formulating drugs, and medicines to overcome the ever-increasing cancer cases around the world is itself a challenge. Using the existing established drugs and increasing their efficacy, sustainability, making it an affordable care against cancer. Herein, we are using a natural drug, artemisinin. Artemisinin is a sesquiterpene that possesses anticancer properties against various cancers. We have synthesized artemisinin-protected iron oxide nanoparticles (ART-IONPs) and investigated their efficacy as a possibility for treating gastric cancer by employing magnetic hyperthermia. The formation of ART-IONPs was confirmed by various characterizations. It is observed from HR-TEM that the particles are spherical in shape with an average diameter of about 7 ± 2 nm. The formulated composite was subjected to FTIR and RAMAN analysis to check the interaction between artemisinin (ART) and iron oxide nanoparticles (IONPs). In addition, we have performed hyperthermia studies to inquire about the heating capacity of the prepared composite. It was observed that it showed a rise in temperature of about 7 ºC at a frequency of 580.3 kHz. Further, the anticancer activity of ART-IONPs was checked on the AGS (Gastric cancer) cell line in the presence and absence of hyperthermia treatment. As a result, it was observed that the formulation has a toxic effect on the AGS cell line, indicating its potential activity as an anticancer agent. This study reveals that artemisinin is a potential therapeutic drug for cancer, and Iron oxide nanoparticles amplify its efficacy with the employment of magnetic hyperthermia. We foresee these ART-IONPs as a promising conjugate for the treatment of gastric cancer.

Keywords: Gastric cancer; Hyperthermia; Artemisinin; Iron oxide nanoparticles; Targeted delivery

Metal-Free, H_2O_2-Mediated, Regioselective Direct C-3 Hydroxylation of Imidazo[1,2-α]pyridines via C(sp^2)-H Bond Functionalization

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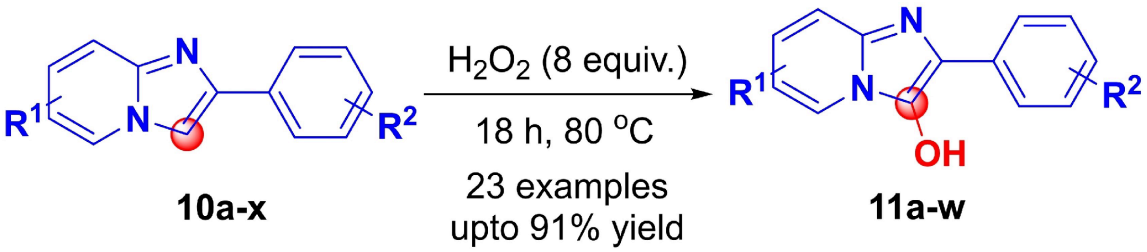
Abstract

Hetero-ring-fused bioactive heterocycles, which are ubiquitous in nature, had received tremendous attention during the last three decades due to its presence in a plethora of pharmaceutically important molecules/therapeutics/drugs.[1–5] Among such bio-heterocycles, imidazo[1,2-*a*]pyridines containing five-membered imidazole moiety fused with six-membered pyridine ring, has been recognized as a "drug bigotry" and are associated with a wide range of biological activities such as antibacterial, antifungal, antiviral, antiprotozoal, antiinflammatory, antitumor, anxioselective activities etc. Imidazo[1,2-*a*]pyridine or its similar skeletal core are also present in several clinically used drugs/therapeutics.

For the first time, a new, cost-effective, metal-free, H_2O_2 (50% in water)-mediated regioselective direct C-3 hydroxylation of imidazo[1,2-*a*]pyridines *via* C-H bond functionalization is reported. This metal-free C(sp^2)-O bond formation protocol is operationally simple and showed broad range of functional group tolerance and substrate affinity. To the best of our knowledge, this is the first report of imidazo[1,2-α]pyridine-3- ols showing promising *in vitro* antioxidant activity.



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