

GLOBAL GROUP OF INSTITUTIONS



**GLOBAL INSTITUTE OF
PHARMACEUTICAL
EDUCATION & RESEARCH**

ADMISSIONS
OPEN



**GLOBAL INSTITUTE OF
NURSING
EDUCATION & RESEARCH**

Jaspur Road, KASHIPUR, Udham Singh Nagar-244713 (Uttarakhand)

Courses Offered at GIPER

D.PHARM

Eligibility - 10+2 with 45% marks
in PCB/PCM

B.PHARM(L.E.)

Eligibility-UKSEE rank holder
or D.Pharm with 1st Division

B.PHARM

Eligibility-UKSEE rank holder or

M.PHARM

(Pharmaceutics &
Pharmaceutical Chemistry)

Eligibility-UKSEE rank holder or
B.Pharm with 1st Division

Courses Offered at GINER

B. Sc NURSING

10+2 with 40% marks
in PCB and English.

G.N.M

10+2 with 40% marks
in English.

Recent Academic Awards:

- Best Pharmacy College in India for Teaching Excellence & Research for Outstanding & Exemplary contribution towards education skill development & research (CEGR) 2023
- Most promising Pharmaceutical Education & Research College in Uttarakhand (WBR), 2023
- Best Pharmacy College in North India (CEGR), 2022
- Best Education Institute with Academic Excellence in India (Eminent Research), 2021

OUR TOPPERS



VAISHALI CHAUHAN
Gold Medalist
B.Pharm,
2013-2017



MONIKA SETIA
Gold Medalist
M.Pharm (Pharmaceutics),
2016-2018



ANKITA SHARMA
Gold Medalist
M.Pharm (Pharm. Chemisry),
2016-2018



GARIMA PANDEY
Gold Medalist
B.Pharm,
2018-2022

100%
PLACEMENTS

Approved by AICTE, PCI New Delhi
& Affiliated to U.T.U. Dehradun &
UBTE Roorkee

Salient Features

- ❖ Modern Computer facility & Wi-Fi Campus
- ❖ Sports & Recreational Activities
- ❖ R&D Environment
- ❖ Lively eco-friendly & lush green campus
- ❖ Enrich Library with 6.5 K standard books, 15 National/International Journals & e-lib facilities
- ❖ Separate training & placement cell
- ❖ CCTV secured campus
- ❖ Focus on personality & holistic development
- ❖ Smart-Class Rooms
- ❖ Sophisticated Laboratories (HPLC, UV-vis, Rota-vap, etc)
- ❖ Well-qualified & experienced faculty awarded with best researcher/Teacher award.



www.giper.edu.in
kmt.giper@gmail.com
kmt.giner@gmail.com

CONTACTS : **9219476108**
8279524911
8534960940

Dream Project of Internationally Renowned Scientists
Only Institute in the region to get OSD
International Collaborations for exchange of students & research



GHTM-2025

INTERNATIONAL SYMPOSIUM ON GLOBAL TRENDS IN HEALTH, TECHNOLOGY & MANAGEMENT

Theme: Innovations and Future Directions in Pharmaceutical Sciences

February 15-17, 2025

Organised By :

GLOBAL HEALTH TECHNO-MANAGEMENT FORUM (GHTMF)
GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION & RESEARCH (GIPER), KASHIPUR (US NAGAR), INDIA



Venue: The Tiger Camp Resort, Ram Nagar, Uttarakhand

Website: conference.ghmtf.com, e-mail: gthtm2025@gmail.com, Ph. +917500458478

Our Sponsors



SOLIZE



entomo



Springer



With best
compliments



SOLIZE



11/12, Udyog Nagar, S. V. Road, Goregaon (W), Mumbai- 400104. Phone: +91.22.67607080
Email: info@themismedicare.com Website: <http://www.themismedicare.com>

With best
compliments



entomo

With best compliments



Pharmaceuticals Pvt. Ltd.

With best compliments



Springer



Shweta Scientific

Deals in : Scientific, Laboratory & Industrial Equipments

B-10, Ramadheen Singh Complex, Faizabad Road, Babujanj, P.O. Nirala Nagar, Lucknow-226020.

Ph. : 0522-2787086
FAX : 0522-4000108

Mob. : 09415080246
09415468967
E-mail : shweta_sci@yahoo.in

CONFERENCES



GTHTM-2025

INTERNATIONAL SYMPOSIUM ON GLOBAL TRENDS IN HEALTH, TECHNOLOGY & MANAGEMENT

Theme: Innovations and Future Directions in Pharmaceutical Sciences

February 15-17, 2025

Organised By :

GLOBAL HEALTH TECHNO-MANAGEMENT FORUM (GHTMF)
GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION & RESEARCH (GIPER), KASHIPUR (US NAGAR), INDIA



Venue: The Tiger Camp Resort, Ram Nagar, Uttarakhand

Website: conference.ghTMf.com, e-mail: gtHTM2025@gmail.com, Ph. +917500458478

Our Sponsors



SOLIZE



entomo



Springer



Patron

Prof. (Dr.) Anil Kumar Saxena, Hon'ble Chairman
Global Institute of Pharmaceutical Education and Research Kashipur, India

Organising Committee

Chairman

Prof. (Dr.) Deepak Teotia

Organising Secretary

Prof. (Dr.) Sisir Nandi

Co-Organising Secretary

Mr. Sarfaraz Ahmed

Members

Mr. Arun Kumar, Mr. Rajan Kaushik, Mr. Muneer Alam, Mrs. Swati Tamta, Ms. Anjali Negi, Mr. Shahjad, Mr. Divyanshu Kumar, Mrs. Vineeta Pandey, Mr. Harsh Sharda, Mr. Raja, Mr. Adil, Mr. Sarfaraj, Mr. Kuldeep Singh, Mr. Rahul Kumar, Mr. Fareed, Mr. Puneet Joshi

International Advisory Committee

Prof. Alain Carpy (CNRS, Bordeaux, France)

Prof. Athina Geronikaki (Aristotle University, Greece)

Prof. Emil Reisinger (University Medical Center, Rostock, Germany)

Prof. Esin AKI-YALÇIN (Ankara University, Faculty of Pharmacy, Ankara)

Dr. Imran Ahmad (Jina Pharmaceuticals Inc, USA)

Prof. Ismail YALÇIN (Ankara University, Faculty of Pharmacy, Ankara)

Dr. James Devillers (CTIS, France)

Prof. Johann Gasteiger (Friedrich-Alexander-Universität, Germany)

Prof. Krishnan Balasubramanian (Arizona State University Tempe, AZ)

Prof. Lakshmi P. Kotra (University of Toronto)

Mr. Ludy Suryantoro (Team lead, Multisectoral engagement, WHO, Switzerland)

Prof. Marjan Vracko (National Institute of Chemistry, Slovenia)

Prof. Om Prakash (Kansas State University, KS)

Dr. Omer Saka (EY Parthenon Health Sciences and Wellness, Switzerland)

Prof. Subhash C. Basak (University of Minnesota, USA)

Prof. Dr. med. Thomas Hohlfeld (University of Düsseldorf)

Dr. Ved Srivastava (Chemistry Intarcia Therapeutics Inc, USA)

Prof. (Dr.) Vladimir Poroikov (Institute of Biomedical Chemistry, Russia)

National Advisory Committee

Dr. Alok Saxena (Advisor, GTC, Vorro Technology, United States)
Prof. B. Jayaram (IIT, New Delhi)
Dr. Dinesh Patel (MD and CEO, Themis Medicare, Haridwar)
Prof. D.S. Rawat (Vice Chancellor, Kumaun University, Nainital)
Prof. Indira Ghosh (Ex- Professor, SCIS JNU, New Delhi)
Prof. Kunal Roy (Professor and Ex-Head Pharmaceutical Technology, Jadavpur University, Kolkata)
Dr. Madhu Dikshit (Ex-Director, CSIR-CDRI, Lucknow)
Dr. O.N. Tripathi (President, The Academy of Life Sciences, Lucknow)
Prof. Poonam Tandon (Vice Chancellor, Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur)
Prof. P.V. Bharatam (Professor and Head, NIPER, Mohali)
Prof. Dr. Rashmi Kumar (Ex- Professor and Head, Department of Pediatrics, KGMU, Lucknow)
Prof. Dr. Sandeep Kumar (Professor & Founder Director AIIMS Bhopal)
Dr. Sanjay Batra (Chief Scientist, CSIR-CDRI, Lucknow)
Prof. Shailendra K. Saraf (Dean (Pharmacy), Dr. APJAKTU & Director (Pharmacy), BBDNIIT, Lucknow)
Prof. Shubhini A. Saraf (Director, NIPER, Raebareli)
Prof. Soniya Nityanand (Vice Chancellor, KGMU, Lucknow)
Prof. T.K. Chakraborty (IISC, Bangalore)
Dr. Vineet Kumar (Scientist-G, Chief Scientist and Professor, Forest Research Institute, Dehradun)
Dr. Yatendra Kumar (Ex-President, Wockhardt)
Prof. Y. K. Gupta (Ex- Head, Dept. of Pharmacology, AIIMS, New Delhi)

Dr. Dhan Singh Rawat
Minister
Medical Health and Medical
Education, Co-operative, Higher
Education, Sanskrit Education,
School Education



Vidhan Sabha Bhavan
Dehradun
Room No. 18
Ph. 0135-2666410 (Off.)
0135-2666411 (Fax)
Mob. 9412370255



MESSAGE

It is my great pleasure to note that **Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur** is organizing an international symposium on "**Global Trends in Health, Technology and Management**" (GTHTM-2025) from **15 to 17 February, 2025**.

It makes an excellent international platform of brain storming scientific sessions for the leading scientists, young researchers, academicians and students globally to discuss the interdisciplinary fields of drug design, discovery and development research. Innovations and Future Directions in Pharmaceutical Sciences to attain the sustainable development goals for the human benefit.

I thank the organizing committee and warm wishes for the success of this symposia.

(Dr. Dhan Singh Rawat)



वीर माधो सिंह भण्डारी उत्तराखण्ड प्रौद्योगिकी विश्वविद्यालय

(उत्तराखण्ड सरकार द्वारा अधिनियम 415/2005 द्वारा स्थापित पूर्ववर्ती उत्तराखण्ड तकनीकी विश्वविद्यालय)

**VEER MADHO SINGH BHANDARI
UTTARAKHAND TECHNICAL UNIVERSITY**
(Formerly Uttarakhand Technical University Established by Act no. 415/2005 by Uttarakhand Government)

Prof. (Dr.) Onkar Singh

Vice Chancellor

प्रो० (डॉ०) ओंकार सिंह

कुलपति

Office Address :

Chakrata Road, P.O. Chandanwari, Premnagar, Suddhowala

Dehradun - 248007, Uttarakhand (India)

Phone No. : 0135-2774068,

Email : vc@uktech.ac.in, Website : www.uktech.ac.in


Ref. No. 223/VC/UTU/25

Date 04-02-2025

Message

I am delighted to know that Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur is organizing an international symposium on "Global Trends in Health, Technology and Management" (GTHTM-2025) during February 15-17, 2025. This conference will provide a platform for brain storming among the leading scientists, young researchers, academicians and students globally. The discussions will pave the way for the advancements in interdisciplinary fields of drug design, discovery and development, innovations and future directions in pharmaceutical sciences and help in the sustainable development.

I congratulate the organizers and extend my best wishes for the successful organization of this symposia.


(Prof. Onkar Singh)
Vice Chancellor



GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION & RESEARCH (GIPER)

D. PHARM, B. PHARM, M. PHARM

Approved by : AICTE & PCI, New Delhi

Affiliated to : UBTE Roorkee and Uttarakhand Technical University, Dehradun

Ref. No.

Date 12/02/2025

Message

It is with great pleasure that we announce that the Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur along with Global Health Techno Management Forum (GHTMF) is organizing the 2nd "International Symposium on Global Trends in Health, Technology, and Management" (GTHTM-2025) in the scenic and serene surroundings of Jim Corbett National Park at The Tiger Camp, Ram Nagar, Uttarakhand during February 15-17, 2025. Building on the tremendous success of GTHTM-2024 where scientists from across the globe including WHO delegates from Switzerland actively participated, the upcoming symposium aims to further extend the initiated valuable discussions. It will also address a wide range of topics, spanning drug design and discovery in the fields of pharmaceutical, medical and biomedical sciences, along with newer technologies involving artificial intelligence in stem cell therapy, microbial resistance, digital and public health.



We are pleased to announce the successful publication of the proceedings from the "International Symposium on Global Trends in Health, Technology, and Management" (GTHTM-2024) by Springer Nature. This achievement reflects the high-quality research and discussions from the symposium, where experts addressed global challenges in health, technology, and management. The proceedings highlight innovative ideas and reinforce the symposium's global impact, serving as a valuable resource for scholars and professionals in these fields. We are excited to continue this collaboration with Springer Nature for GTHTM-2025. This continued collaboration with a prestigious publishing house underscores the significance of the event and its contributions to advancing knowledge in these critical areas.

This International Symposium serves as a venue to unite stakeholders from diverse disciplines to share ideas and work together for societal progress. I hope that the discussions here will focus on translating the advancements in these areas into tangible benefits for the general public, improving health and the environment, with GIPER and GHTMF playing a key role in this effort.

I warmly welcome all participants and look forward for their active involvement in ensuring the success of this event. I also wish to express my gratitude to the distinguished scientists, educators, business leaders, and professionals for honouring us with their presence. My sincere appreciation goes to the organizing committee, staff, and students of GIPER, Kashipur, for their dedicated efforts. I am confident that this event will be a great success.

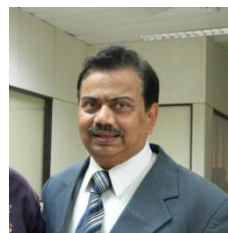
Anil Kumar Saxena

Dr. Anil Kumar Saxena
Chairman

BIOGRAPHIES OF RESOURCE PERSONS

Dr. A. K. Dwivedi

Dr. A.K. Dwivedi is presently consultant (Phytopharmaceutical Mission). He was former Head and Chief Scientist of Pharmaceutics Division, Central Drug Research Institute, Lucknow, India. He accomplished his basic education viz. graduation and post-graduation along with doctorate from Agra University, Agra. During 1992-1993 he was on deputation at Aston University, Birmingham, U.K. for research activities. He was again on deputation at Bradford University, Bradford, U.K. in 2010 and Greece in 2015. Till date he has 85 patents and 4 Technology Transfers to this name. So far, he has contributed in 140 different internationally peer-reviewed journals.



Dr. Aaruni Saxena

Dr Aaruni Saxena is a clinician with an interest in the management and development of health plans and policies related to global health security. He completed his medical graduation and doctoral studies in medicine from the University of Rostock and Heinrich Heine **University Düsseldorf**, Germany. Later, he was awarded a prestigious United Nations fellowship for a Master of Business Administration at the University of Geneva, Switzerland. He is also a recipient of the Swiss Fellowship for Infectious Disease, Basel. He completed his specialist training in Acute Internal Medicine and holds a Membership of the Royal College of Physicians, United Kingdom. He has worked as a technical consultant to the World Health Organization as an adviser on health emergency preparedness. He has a good number of high-impact national and international publications with more than 100 citations. At present, he is working as a consultant in NHS, United Kingdom.



Dr. Anil Kumar Saxena

Dr. Anil Kumar Saxena, honorable Chairman, Global Institute of Pharmaceutical Education and Research, and Ex-Chief Scientist and Head, Medicinal and Process Chemistry Lab, CSIR Central Drug Research Institute, India is actively involved in Medicinal Chemistry & Computer Aided Drug Design (CADD). He has more than 50 years of research experience, 270 research papers, 50 reviews/articles in books/monographs and 72 patents to his credit. He has delivered >200 invited lectures, chaired >100 session and has been visiting the globe for research presentation. He has supervised >200 post graduates and 46 PhD students. Dr. Saxena has initiated QSAR and the concepts of CADD in early 70's and father of QSAR in India and abroad. He is recipient of several awards, including Alexander von Humboldt Fellowship, INSA Young Scientist Medal, Themis Chemicals UDCT Diamond



Jubilee Distinguished Fellowship, Ranbaxy Research Award in Pharmaceutical Sciences, and many more. He is the Editorial Board Member of different prominent journals like, Medicinal Chemistry Research, SAR and QSAR in Environmental Research, Current Topics in Medicinal Chemistry and online international journal ARKIVOC. It is noteworthy that Dr. Saxena has been enlisted for the 4th consecutive year in the list of the top 2% scientist in the world Stanford University, USA.

Dr. Alok Kumar Saxena

Alok Saxena superannuated as Managing Director, Sulzer GTC India Pvt. Ltd and presently is proprietor of AA Consultants. He is a Chemical Engineer with Doctorate from IIT, Delhi and Post-Doctorate from University of Oldenburg, Germany. He more than 44 Years of experience covering assignments as: Deputy Director, Indian Institute of Petroleum, Dehradun, Chief R&D Manager-BPCL, General Manager, Process Licensing for Axens in India, Professor at UPES Dehradun. Significantly contributed in the development of refining technologies and commercialization through close R&D and process design interaction, modeling and simulation, scale-up from lab scale concepts to commercial design. He has more than 50 publications in journals / encyclopedia and conferences and has 4 patents. Dr. Saxena is a recipient of CSIR Young Scientist Award in Engineering Sciences and CSIR Technology Awardee.



Dr. Asmita Samadder

Dr. Asmita Samadder is working as an Assistant Professor, Department of Zoology, University of Kalyani, India. Her H index is 33, i-10 index: 50. She worked in an International Project, from Lyon France, during her PhD tenure, and later completed her training at Jawaharlal Nehru University, New Delhi, India, as DST Postdoctoral fellow in Nanoscience and Technology. She has over 100 original research publications in international peer-reviewed journals of repute. Dr. Samadder works in the area of Nanotechnology and nano-medicine more than 17 years. Her research interest includes nano-formulation of several drugs to combat Diabetes and its associated complications like Alzheimer's disease, diabetic kidney diseases, etc, along with other toxicological pathophysiology under research grant of SERB (DST) and UGC Govt. of India. She is the winner of "Young Scientist Award" in SYDNEY and Je Ma award SWEDEN. She is the Editorial Board member of several internal journals like, Journal of Cellular Biological and Molecular, Sciences, International Journal of Experimental Research and Review, Nano and Medical Material and many more.



Prof. Athina Geronikaki

Prof. Athina Geronikaki graduated from Tashkent State University in 1971 and gained the specialty of organic chemist. In 1977, she received the Doctor of Philosophy in Chemistry. In 1984, she graduated from School of Pharmacy of Aristotelian University of Thessaloniki. From 2006-2016 she was the Head of the Department of Pharm. Chemistry. Since 2010 she is Full Professor of Medicinal Chemistry of School of Pharmacy of Aristotle University of Thessaloniki. During 2009-2011 she was Vice President of School of Pharmacy of Aristotle University of Thessaloniki. In July 2013 Prof. Geronikaki was elected as a Full member of Mediterranean Academy of Science and Arts and in 2015 Member of European Academy of Science and Arts. She has been working on drug design and synthesis and screening of bioactive compounds. She is the member of CMTPI and organized many international conferences like Computational Methods in Toxicology and Pharmacology, Internet Integrating Resources (CMTPI) (2003); 4th Eurasian Meeting on heterocyclic Chemistry 2006, 8th CMTPI -2015 and 23d Hellenic Symposium in Medicinal Chemistry, 2017, CMTPI-2019. She published more than 200 papers and 5 chapters in a book. Wrote 4 books for student. She has 23 Erasmus agreements and is University coordinator of Paul Ehrlich PhD Network in Medicinal Chemistry. She is member of Editorial Board in several journals such Molecules, Jordanian J. of Chemistry, International Journal of Pharmaceutical Sciences Research, Diabetes & obesity International Journal, Journal of Drug Design and Research, and Executive editor in Current Topics in Medicinal Chemistry.



Prof. B. Jayaram

Prof. B. Jayaram received his Ph.D. in 1986 from the City University of New York. He then worked as a Post Doctoral Fellow (1987-88) with Prof. Barry Honig at Columbia University, USA and as a Senior Research Associate (1989-1990) at Wesleyan University, USA. In 1990, Prof. Jayaram joined IIT Delhi and later had been Head of Chemistry Department, IIT Delhi (2006-2009), he is Founder Coordinator of Kusuma School of Biological Sciences, Supercomputing Facility for Bioinformatics & Computational Biology (SCFBio), IIT Delhi. Prof. Jayaram served as a member of many prestigious committees. He guided 30 PhD students and dissertations of several M. Tech. and M.Sc. students. Prof. Jayaram is responsible for the creation of science and software of Chemgenome, the genome annotation software, Bhageerath, the protein structure prediction website, Sanjeevini, the computer aided drug design software suite, the Dhanvantari (Genome Drug pathway) suite and several other molecular modelling and bioinformatics utilities, and making these software tools freely accessible to the global user community through scfbio website (www.scfbio-iitd.res.in). Prof. Jayaram is currently Mentor, SCFBio, IIT Delhi (2023-2027).



Professor Diwan S. Rawat

Professor Diwan S. Rawat, is a Vice Chancellor of Kumaun University from where he did his masters in 1993. After obtaining his Ph.D. from Central Drug Research Institute, Lucknow he worked at Indiana University and Purdue University, USA as a postdoctoral fellow. He was an Assistant Professor for a short period of at NIPER, Mohali and joined Delhi University in 2003. Prof. Rawat has published over 170 research papers, authored a book, five book chapters, and eleven patents to his credit. His research work has been cited over 6900 times with impressive h-index of 49 and i-10 index of 132. One of his compounds has entered Phase I clinical trials for the Parkinson treatment. Prof Rawat has supervised 27 PhD students. His Parkinson work has been published by NATURE COMMUNICATION. He was elected as President of Chemical Sciences Section of Indian Science Congress (2019-20) and he is a Visiting Professor at Japan Advanced Institute of Science and Technology. He has been awarded many prestigious awards.



Dr. Disha Dutta

Dr. Disha Dutta is an accomplished academician with over 17 years of experience in pharmaceutical education and research. Currently serving as Professor at Devsthali Vidyapeeth College of Pharmacy, Rudrapur, Uttarakhand. She has mentored numerous M. Pharm students and specializes in Pharmaceutics, her area of interest is Cosmetology and novel drug delivery systems. She has delivered guest lectures, including a DBT-associated talk on COVID-19 treatment innovations and a session at Sage University on biosensors in disease diagnosis. Dr. Dutta has authored books on Pharmaceutical Engineering and CADD and contributed to book chapter on Microbes in the Baking Industry: Harnessing the Power of Microbes in Baking Products, Springer Nature. With over 25 research publications in reputed journals and multiple patents in drug delivery and immunomodulation, she is actively engaged in learning and innovation. A lifetime member of APTI and an approved PCI Inspector.



Professor Gunda Georg

Professor Gunda Georg earned a B.S. in pharmacy and a Ph.D. in Medicinal Chemistry from Philipps Universität Marburg, Germany. After postdoctoral studies (University of Ottawa in Canada), she became a faculty member in the Department of Medicinal Chemistry at the University of Kansas. In 2007, she joined the University of Minnesota Department of Medicinal Chemistry and leads the Institute for Therapeutics Discovery and Development. She was Editor-in-Chief of the Journal of Medicinal Chemistry (2012-2020). She is an AAAS Fellow and an American Chemical Society Fellow.



In 2017, she was elected to the Hall of Fame of the Medicinal Chemistry Division of the American Chemical Society. In 2020, she received the Alfred Burger Award in Medicinal Chemistry from the American Chemical Society and, in 2023, the Carl Mannich Medal from the German Pharmaceutical Society. Her research interests are medicinal chemistry, drug discovery, contraception, and cancer. She is co-inventor of one marketed drug and three drugs in clinical trials. She has published 270 articles, has 13,043 citations, and an h-index of 61 (January 2025). She has trained over 100 students, postdocs, and visiting scientists.

Prof. Indira Ghosh

Prof. Indira Ghosh is working in JNU since 2008 as Dean & Professor to steer the School of computational & integrative sciences, which deals with computational approach to Biology, Chemistry, and Economics etc. She has nourished the school as Center of Excellence under Department of Biotechnology in Computational Biology and spearheaded to initiate a new stream supported by UGC, called complex systems, harvesting few faculties from Physics and Econophysics. She has been one amongst the earlier scientists to realize the importance of Bioinformatics and initiated M.Sc courses in Pune University (SPPU) when she joined as Professor in Institute of Bioinformatics & Biotechnology in Pune in 2003. She published one of the first Docking algorithms in early eighties as a part of her thesis and developed difference of Free Energy calculation method in Biomolecules during her post-doc. Her major contributions are to develop and contribute in the field of Bio & Chemoinformatics, using Systems Biology approach to find pathway & target enzymes and developing novel tools for molecular simulations and pharmacophore design using known protein structure. She has guided 12 Ph.D, 5 M. Tech & 20 M.Sc students, mentored 7 Research Associates since last 15 years (academic) to direct them towards the evolving field of Computational Biology. During 2003-2017 She has completed 12 projects supported by IBM, DBT, IUTSSF & DeITY, some of them have potential to collaborate with industry and has published 65 papers as communicating author. During last 15 years she has been servicing as member or chair of Bioinformatics task forces in DBT, Ministry of Electronic Communication & Information Technology) and ICMR respectively.



Dr. Lakshmi P. Kotra

Dr. Kotra is an academic entrepreneur with expertise in drug discovery and development. Kotra group specializes in the areas of medicinal chemistry, preclinical and clinical development of small molecule and natural product-based drugs. Dr. Kotra authored/co-authored over 135 peer-reviewed articles and book chapters, and delivered over 150 scientific and plenary talks globally. Kotra research group has contributed to a number of research programs in the areas of infectious, metabolic and neurodegenerative diseases, cancer,



thrombocytopenia among others. Dr. Kotra is a recipient of several awards including the Premier's Research Excellence Award from the Province of Ontario (Canada), Rx&D Health Research Foundation Research Career award, GlaxoSmithKline/Canadian Society for Pharmaceutical Sciences Young Investigator Award. His accomplishments include discovery and development of drug candidates/dietary supplements from discovery to clinical development to market for multiple sclerosis (Lucid-21-302), malaria (Kopakamal), diabetic neuropathy (WST-052) and acute alcohol intoxication (marketed product, unbuzzd™). Dr. Kotra is a co-founder of WinSanTor Inc., San Diego, California, USA (drugs targeting diabetic neuropathy, and many more).

Dr. R. Natarajan

Dr. R. Natarajan Completed M.Sc. in chemistry in 1979 from St Joseph's College and finished Ph.D. in Chemistry from Bharathidasan University, Tiruchirappalli, Tamil Nadu in the year 1995. From 2004-07 worked as a Scientist in Dr Subhash Basak's group at Natural Resource Research Institute, USA. From 2010 to 2019 worked as the CEO of a polymer company in Karur, Tamil Nadu. During this period, he developed three vector control products namely chemically treated mosquito nets that are recommended by World Health Organization to be used in controlling malaria transmission. This contribution enabled the industry in earning 40 million US dollars per annum and provided jobs for more than 3000 employees of Karur district in Tamil Nadu, India. Returned to academia in 2020 at present working as head, research and development in Saranathan College of Engineering, Tiruchirappalli. He Published more than 45 research papers, written book chapters and review articles. Visited more than 20 countries and presented research papers.



Mr. Prakhar Saraswat

Prakhar Saraswat having MBA, M.Tech and B. Tech degrees, is a dynamic and results-driven professional with over 13 years of experience in the IT industry, excelling in delivery, stakeholder management, and leadership roles. Throughout his career, Prakhar has consistently demonstrated a strong ability to lead cross-functional teams, manage large-scale projects, and drive digital transformation initiatives. His expertise lies in implementing innovative solutions, optimizing business processes, and fostering operational excellence to enhance efficiency and scalability. In his current role as Head of Operations, Prakhar spearheads process automation and strategic optimization, ensuring seamless execution while driving continuous improvement. His keen focus on leveraging technology, data-driven decision-making, and organizational agility enables businesses to stay ahead in an evolving digital landscape. With a proven track record of leadership, execution, and innovation, Prakhar remains committed to empowering organizations with transformative strategies that fuel sustainable growth and success.



Dr. Shubhra Ghosh Dastidar

2005: PhD in Chemistry from University of Calcutta

2005-2010: Postdoc in UCDavis, UTexas at Galveston and A*STAR(Singapore), has worked with eminent scientists like Yong Duan, Chandra Verma.

2011: Joined Bose Institute as Assistant Professor

At present, working as a Professor, in the Department of Biological Sciences.

Area of Specialization is the investigation and understanding of the molecular mechanisms of functions of Biomolecules and their complexes from the perspective of a theoretical chemist, using computational methods, particularly starting with simulation of structural dynamics with the use of large-scale high-performance computing facilities. Some of his favorite systems are Tubulins, Bcl2 family of proteins, Kinases etc. Serving as the coordinator of the DBT funded Bioinformatics centre project at Bose Institute and also as the multi-institutional National Network Project. Published 46 papers so far, all in internationally reputed journals. Currently is an Associate Editor of the Frontiers in Molecular Biosciences.



Prof. (Dr.) Sisir Nandi

Prof. (Dr.) Sisir Nandi completed Ph.D. from Indian Institute of Chemical Biology (CSIR) as a CSIR-GATE fellow, India and had been awarded Ph. D. in Pharmacy degree (2010) by the Jadavpur University, India. He did his post-doctoral research as the European Union Marie Curie fellow in National Institute of Chemistry, Ljubljana, Slovenia. Dr. Nandi is working in the area of QSAR, anti-

COVID-19, anticancer, antiviral, antitubercular, antimalarial drug design, development and discovery research, biological activity prediction of lead compounds, ligand-receptor interactions, virtual screening, combinatorial library design and lead-hopping. He published more than 150 original research articles and reviews in reputed international journals having high impact factor. He published 10 book chapters in Springer Nature and Bentham book. He presented his research work in many international conferences around Europe. He is Editorial advisory board members of Scientific Reports (Nature); Discover Chemistry (Springer), Trends in Advanced Sciences and Technology and many reputed journals. He is having more than 15 years of teaching and 20 years of research experiences. He has been guiding many master's and doctoral students. He is very competent in organizing many Govt funded international seminar, conferences and symposia as organizing Secretary (CPDDP-2014, CMTPI-2017; CTPMS-2020, DDDR-2021, GTHTM-2024 and 2025). He has been working with government funded research projects.



Prof. Dr. Soniya Nityanand

Prof. Dr. Soniya Nityanand, honorable Vice Chancellor of King George Medical University, Lucknow, is an immunologist specializing in hematology. She did her graduation and post-graduation both from King George's Medical College, Lucknow. She later went on to pursue her PhD in Immunology from Karolinska Institute, Stockholm, Sweden in 1996.



In the initial phase of her career, Nityanand worked as an Assistant Professor in medicine in KGMC, Lucknow where she served from October 1991 to November, 1993. After that, she has been a faculty member at SGPGIMS from Nov 1993, initially in the Dept of Immunology and recently in the Dept of Hematology. She has also been a visiting fellow in immunology and hematology at Karolinska Institute, Stockholm in the year 1991–1992.

In 2021, she was appointed as director of Dr. Ram Manohar Lohia Institute of Medical Sciences. Prof. Dr. Nityanand is honorable vice chancellor of King George's Medical College, Lucknow.

Prof. Nityanand is recipient of several awards such as

- Department of Biotechnology National Bioscience Award for Career Development for 2003–04.
- Indian National Science Academy Young Scientist Award for 1990.
- Dr JC Patel and BC Mehta award of the Association of Physicians of India for 2000.
- Dr NN Gupta Gold Medal
- Chancellor's Medal for the best Medical Student.

Dr. Srikanta Kumar Rath

Srikanta Kumar Rath is chief scientist and professor of AcSIR-CDRI. He is a very potent Molecular and Cell Biology researcher with more than 30 + years of research experience in a large academic institution, leading to diverse scientific projects. Extensive hands-on training and experience in the area of protein biochemistry, molecular biology, cell biology, microscopy, and Cell Biology. Experience in designing experiments and data analysis. Knowledge in various biochemical, molecular, and Life Sciences techniques. He has diverse Expertise on Gene Expression, PCR, DNA, Cell Culture, Cancer Biology, Sequencing, RNA, Molecular Genetics, Immunohistochemistry, and Cloning.



Dr. Subhash C. Basak

Dr. Subhash C. Basak is a retired Adjunct Professor in the Department of Chemistry and Biochemistry, University of Minnesota USA. He received his PhD in biochemistry in 1981 from the university of Calcutta, India. His current research interests involve discrete mathematical chemistry and its applications to chemoinformatics, bioinformatics, quantitative structure-activity relationship (QSAR), computational toxicology, mathematical quantification of DNA/ RNA sequences, mathematical proteomics, and computer-aided vaccine design for emerging pathogens like Zika virus, COVID-19. Dr. Basak is the former Editor-in-chief of Current Computer Aided Drug Design. He has been published many books. Dr. Basak has authored more than 400 papers and book chapters. He received a total of US\$7,466,017 in grants and contracts. He is the past President of the international society of mathematical chemistry and a member of the international academy of mathematical chemistry (IAMC). He is the founder Chairperson of three mathematical chemistry conference series involving India, USA and countries of South America.



Prof. Dr. Vladimir Poroikov

Vladimir Poroikov is the Principal Researcher and Head of Department for Bioinformatics & Laboratory for Structure-Function Based Drug Design at the Institute of Biomedical Chemistry, Moscow, Russia. Graduated as M.Sc. in Physics (1974) and earned his Ph.D. degree in Biophysics at the M.V. Lomonosov Moscow State University (1981). Dr. Sci. (Pharmacology, 1995). Professor (Biochemistry, 2000), Professor (Mathematical Biology & Bioinformatics, 2013), Correspondent Member of Russian Academy of Sciences (Medical Bioinformatics, 2019).



Member of the Council for Grants of the President of the Russian Federation, Expert of Skolkovo Foundation, Russian Academy of Sciences, Ministry of Education and Science, Russian Science Foundation and Russian Foundation of Basic Research. Member of the American Chemical Society, Russian Biochemical Society; Society of Russian Pharmacologists. Editorial Board Member: Big Data Mining and Analytics, Biomedical Informatics, SAR and QSAR in Environmental Research, Biomedical Chemistry, Pharmaceutical Chemistry Journal. Co-author of 350+ publications in the peer-reviewed journals and book chapters with about 8,000 citations (H-index 41). Keynote Speaker of over 20 International conferences and symposia in 2021-2024. Supervision: 2 Doctor of Sciences, 16 PhDs; 20 Graduate Students.

Research interests: Bioinformatics, Chemoinformatics, (Q)SAR, Molecular Modelling and Computer-Aided Drug Design & Discovery.

Prof Y K Gupta

Dr. Y.K. Gupta M.B.B.S (1974), M.D (Pharmacology, 1979) from King George's Medical College, Lucknow, is President of AIIMS, Jammu, former Professor and Head, Department of Pharmacology and Spokesperson, All India Institute of Medical Sciences (AIIMS), New Delhi. He earlier served as Sub Dean, AIIMS (1996 – 2001). and Director, Indian Institute of Toxicology Research (IITR, CSIR), Lucknow from 2003 to 2005. Dr. Gupta is in charge of National Poison Information Centre and is also National Scientific Coordinator of Pharmacovigilance Program of India (PvPI). He has been honored with fellowships of National Academy of Medical Sciences (FAMS), Indian Pharmacological Society (FIPS), National Academy of Science (FNASc), Indian Academy of Neurosciences (FIAN) and Society of Toxicology (India) (FST). He has more than 180 publications in International and National journals and several chapters in books to his credit. Dr Gupta is recipient of several awards including Young Scientist Medal from Indian National Science Academy, Shakuntala Amirchand Prize (Indian Council of Medical Research : ICMR), Chandrakanta Dandiyia Prize, G. Achari Oration Award (Indian Pharmacological Society : IPS), Major General S. L. Bhatia Oration Award (Association of Physiologist and Pharmacologist of India : APPI), AEB Honours Award (Academy of Environmental Biology), C. L. Malhotra Prize (Association of Physiologist and Pharmacologist of India : APPI) etc. Dr. Gupta is currently President of Society of Toxicology, India and Dean Indian Society for Rational Pharmacotherapeutics, and was President of the Indian Pharmacological Society (2005- 2006). He is the Editor of the Indian Journal of Physiology and Pharmacology (Pharmacology Section) and member editorial board of several International and Indian journals. He is the Chairman of National Committee of IUPS-IUPHAR of Indian National Science Academy (INSA), Member of IUPHAR –IOSP committee and member of Advisory Committee on Safety of Medicinal Products (ACSoMP) of WHO, chairman of Equivalence Committee and member Ethics Committee of Medical Council of India. He has been member of Project Advisory Committee / Research Council / Scientific Advisory Committee and Task force of CSIR, ICMR, DST and DBT and Chairman, SAC of National Institute of Occupational Health (NIOH-ICMR). He is chairman of national GLP technical committee of DST, member of the Scientific Body of Indian Pharmacopoeia (IP) and Chairman of Expert Committee on Clinical Medicine and Pharmacology of IP. He was the Governing body member of Indira Gandhi Postgraduate Institute of Medical Education and Research, Patna. He was the Chairman of National Essential Medicine List Committee 2011 of Ministry of Health & Family Welfare, Government of India and also the Chairman of the working group of High Powered Inter-Ministerial Coordination Committee to look into the matters of implementation Government commitment to provide quality medicine at affordable prices.



ABSTRACTS OF RESOURCE PERSONS

**REFRACTORY HYPERCALCEMIA IN NEUROENDOCRINE TUMORS:
DISCORDANCE BETWEEN HISTOLOGY AND IMAGING IN TUMOR
PROGRESSION**

*Arora Jitesh**, *Aithal Guru***, *Chauhan Vishnusai**, *Kaye Philip**, *Dharani Medonsa**
*Shah Meetal**, *Gangi Anmol**, *Gomez Dhanny**, *Syed Monawer karem**, ***Saxena Aaruni****

*Nottingham City Hospital, University of Nottingham, United kingdom

** NIHR Nottingham Biomedical Research Centre, Nottingham University Hospitals NHS
Trust and the University of Nottingham

Neuroendocrine tumours (NETs) are rare malignancies often presenting with diagnostic challenges. This case discusses a 62-year-old male with hypercalcemia and acute kidney injury in May 2024. Imaging played a crucial role in diagnosing and characterizing the tumour. Initial CT scans revealed a large retrosternal thyroid goitre and extensive liver deposits, raising suspicion of metastatic disease. Octreotide scans confirmed somatostatin receptor expression, while FDG-PET imaging showed widespread metastasis, with high uptake in the sigmoid colon, suggesting a likely colonic primary. Further imaging identified new lung nodules, extensive liver metastases with necrotic cores, pleural effusions, and vascular encasement, indicating aggressive disease progression. The discordance between octreotide and FDG-PET uptake in the sigmoid mass raised concerns about de-differentiation or tumour heterogeneity. Although initial biopsy was reported as well-differentiated NET but subsequent re-review was carried out due to FDG-PET positivity and radiological progression, which revealed areas of poor differentiation NET, with high Ki-67 index, correlating with the tumour's aggressive behaviour. Based on the FDG-PET findings, the patient was treated with carboplatin and etoposide starting in July 2024, but despite initial response, recurrent hypercalcemia episodes delayed further chemotherapy. Cinacalcet was introduced, but electrolyte abnormalities led to discontinuation of chemotherapy, and rapid disease progression occurred. This case illustrates how refractory hypercalcemia, coupled with discordant imaging and histological findings, may suggest tumour heterogeneity, complicating diagnosis and treatment in NETs.

INNOVATIONS IN DRUG DESIGN: CASE STUDIES FROM DISCOVERY TO DEVELOPMENT

Anil Kumar Saxena

Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research, Jaspur Road, Kashipur, Uttarakhand

Drug design is a critical aspect of drug discovery and development, a complex, costly, and time-consuming process aimed at identifying promising drug candidates for human therapeutics. The process consists of two main stages: first, the identification of both the target and the lead molecules, and second, the more challenging step of optimizing the lead molecule to develop a candidate drug. Approaches to drug design are essential in both discovering new leads and optimizing existing ones. Traditionally, lead identification relied on natural products, understanding disease mechanisms, random screening, and human pattern recognition. However, the advent of Computer-Aided Drug Design (CADD) techniques has significantly eased the challenges in drug discovery. These methods, based on ligand- and structure-based approaches, involve developing predictive models using tools like QSAR (Quantitative Structure-Activity Relationship), pharmacophores, and docking studies with CAMM (Computer-Aided Molecular Modeling Techniques). These models enable efficient virtual screening, facilitating the identification of lead molecules from vast molecular databases, including focused libraries. CADD also shows promise in repositioning existing generic drugs, which could be particularly beneficial for the Indian pharmaceutical industry. Once suitable leads are identified, they can be further optimized using CADD to address challenges encountered during preclinical and clinical trials, ultimately providing effective drug candidates and new leads. The approaches significantly shorten the timeline from the initial identification of the lead molecules to the selection of the candidate drugs and have been successfully applied in the development of neuroleptics, antihypertensive drugs, anti-Alzheimer's, and antitubercular agents.

CURRENT TRENDS IN HEALTHCARE TECHNOLOGY

Alok Kumar Saxena

AA Consultants

With the rise of Artificial Intelligence (AI), all sectors are poised for significant transformation and evolution of new business models. Pharmaceutical and healthcare industries are no exception to it. While the pharma sector has faced challenges in recent years, which have slowed the adoption of new technologies, it is now positioning itself for substantial change. These changes are necessary to address current issues such as the need for cost-effective medicines, their shortages, sudden demand fluctuations, and the sustainability of long-term business models.

Emerging trends in healthcare technology include:

- **Remote Consultation and Monitoring** through telehealth and telemedicine platforms.
- **Internet of Medical Things (IoMT)**, driven by wearable devices and connected sensors for continuous patient monitoring.
- **Artificial Intelligence (AI)** enabling predictive analytics and early detection of health conditions.
- **Advanced Technologies** such as simulations for medical procedures, pills with internal monitoring capabilities, and targeted treatments using nanomedicines.
- **Remote Patient Monitoring** systems designed to ease the burden on healthcare facilities.

This paper provides an overview of these key trends reshaping the pharmaceutical and healthcare sectors.

MACHINE LEARNING TECHNIQUES FOR BREAST CANCER DIAGNOSIS

Anushree Sinha

Software Engineer, Google LLC, Mountain View, CA

Email: anushreeanushree@gmail.com

Breast cancer remains a leading cause of mortality among women worldwide, emphasizing the critical need for early and accurate diagnosis to improve treatment outcomes and survival rates. This study focuses on developing robust machine learning models for breast cancer prediction using the publicly available Breast Cancer Wisconsin (Diagnostic) dataset. This dataset, comprising features extracted from fine-needle aspirate (FNA) images of breast masses, offers valuable insights into cellular characteristics associated with malignancy.

Our research employs a comparative approach, utilizing a variety of machine learning algorithms, including logistic regression, decision trees, and random forests, to construct predictive models. Each model is trained and evaluated on the dataset, with performance assessed through key metrics such as accuracy, precision, recall, and F1-score. By comparing the effectiveness of these different models, we aim to identify the most suitable approach for accurate breast cancer prediction.

This analysis not only contributes to the expanding field of machine learning in healthcare but also holds the potential to assist clinicians in making more informed diagnostic decisions. The results of this study may pave the way for developing more sophisticated tools to aid in the early detection of breast cancer, ultimately contributing to improved patient care and disease management.

Keywords: Breast cancer, machine learning, diagnosis, prediction, FNA images.

DESIGN, SYNTHESIS AND THERAPEUTIC EXPLORATION OF NANO-BASED PHYTOCOMPOUNDS FOR TARGETING PROTEINS TO COMBAT DIABETES AND ITS COMPLICATIONS

Asmita Samadder

Cytogenetics and Molecular Biology Laboratory, Department of Zoology, University of Kalyani, Kalyani, Nadia 741235, India

Diabetes is a serious metabolic disorder, which has become alarming worldwide. Potential medication for combating the disease has its own set of drawbacks ranging from dose dependency to occurrence of side effects, which has inclined towards usage for natural phyto-compounds. Molecular docking based *in silico* prediction of target protein related to diabetes led towards selection of certain phyto compounds for experimental investigations. Further, design and synthesis of nano-particles using the *in silico* screened phyto-compounds as core materials enhances the activity of the drug pertaining to their bioavailability, targeted delivery and potential binding affinity with proteins. In this study, the selected phyto compound(s) was encapsulated in a biodegradable, non-toxic polymer poly-lactide-co-glycolide (PLGA) to form nano-particles (Nps) which were characterized through AFM, FESEM, DLS, XRD and FTIR studies which confirmed its average size, negative zeta potential, smooth surface area and purity in nature. The overall experimental findings in experimental model demonstrated that Nps significantly delayed diabetes onset by mitigating oxidative stress, genotoxicity, and mitochondrial dysfunction by modulating protein expression by virtue of improve drug solubility and effectivity, targeted delivery, bioavailability, and controlled release of drug from the nano-capsule. Thus, this study suggests a therapeutic possibility of Nps for addressing diabetes and its complications by targeting/ hyper-activating the function of different proteins and modulating other signalling cascades involved therein for providing a better life of diabetics in near future.

Keywords: Diabetes, *in silico* prediction, nano-particles, experimental model

EVALUATION OF 2-PHENYLTHIAZOLIDIN-4-ONE ANALOGUES AS INHIBITORS OF THE SARS-COV-2 MAIN PROTEASE

Anthi Petrou^{1,*}, *Athina Geronikaki*^{1,*}, *Hathaichanok Chuntakaruk*^{2,3}, *Leentje Persoons*⁶, *Thanyada Rungrotmongkol*^{2,3}, *Dominique Schols*⁶, *Aliki Papadimitriou-Tsantarliotou*⁴, *Ioannis S. Vizirianakis*^{4,5}, *Steven De Jonghe*⁶ and *Fliur Z. Macaev*⁷

¹ School of Health, Department of Pharmacy, Aristotle University of Thessaloniki, 54124, Thessaloniki, Greece; geronik@pharm.auth.gr (A.A.); anthi.petrou.thessaloniki1@gmail.com (A.P.).

² Program in Bioinformatics and Computational Biology, Graduate School, Chulalongkorn University, Bangkok 10330, Thailand;

³ Center of Excellence in Structural and Computational Biology, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand; hathaichanok.chuntakaruk@gmail.com

⁴ Laboratory of Pharmacology, School of Pharmacy, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece; ivizir@pharm.auth.gr (I.S.V.); alikipapadi@pharm.auth.gr (A.P-T).

⁵ Department of Health Sciences, School of life and Health Sciences, University of Nicosia, CY-1700 Nicosia, Cyprus.

⁶ Laboratory of Virology and Chemotherapy, Rega Institute for Medical Research, Department of Microbiology, Immunology and Transplantation, KU Leuven, Herestraat 49, P.O. Box 1043, B-3000 Leuven, Belgium leentje.persoons@kuleuven.be (L.P.); dominique.schols@kuleuven.be (D.S.); steven.dejonghe@kuleuven.be (S.D.J.)

⁷ Laboratory Organic synthesis, Institute of Chemistry, Moldova State University, Academiei str., 3, MD-2028 Chişinău, Moldova fliur.macaev@sti.usm.md (M.F.Z.)

The persistence of SARS-CoV-2 mutations contributed to the COVID-19 epidemic's duration and raised concerns about the efficacy of the available vaccines. Herein, we report the evaluation of several thiazole/benzothiazole based thiazolidinone derivatives selected from 85 designed derivatives through docking studies, as potential inhibitors of the SARS-CoV-2 main protease (MPro). The experimental results revealed that out of the fifteen compounds studied, five displayed inhibitory effects with IC₅₀ values ranging from 0.19 to 13.15 µM. The most potent MPro inhibitors were further evaluated for their antiviral efficacy against the delta and omicron variants of SARS-CoV-2. Although certain analogues exhibited antiviral activity, no clear correlation with the MPro inhibition was observed.

TOWARDS MOLECULAR AYURVEDA

B. Jayaram

Supercomputing Facility for Bioinformatics and Computational Biology (SCFBio),
Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India.

Email: bjayaram@chemistry.iitd.ac.in

Structure based drug discovery research has matured to a stage where one can expect lead molecule predictions from computational pipelines to routinely sail through experimental *in vitro* validations. The methods for finding a small molecule inhibitor for a biomolecular target are firmly entrenched. From a molecular perspective, handling multiple drugs binding to multiple targets, some as activators and some as inhibitors, in varying solvent media is what we must be geared upto for simulating a successful Ayurvedic treatment. The talk will discuss the tools already available on the table such as Sanjeevini (<http://www.scfbio-iitd.res.in/Sanjeevini/index.php>) for CADD and BIMP (<https://scfbio.iitd.ac.in/bimp>), a database of 105,909 Phytochemicals found in 6,209 Indian medicinal plants and attempts to sketch a pathway to bridge the gap between modern medicine and traditional Indian medicine.

ONE STEP FORWARD FOR THE DEVELOPMENT OF DRUG FOR NON-CURABLE DISEASE: CLEARANCE OF PHASE I HUMAN CLINICAL TRIALS

Diwan S. Rawat

Senior Professor of Chemistry, University of Delhi and Vice Chancellor, Kumaun University, Nainital, Uttarakhand

The ‘one drug, multiple targets’ concept has gained attention of both the academic and the pharmaceutical industry in recent years. To achieve such goals concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule.^{1,3} 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.⁴ We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine pharmacophore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studied 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.⁵⁻⁸ 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 cure the Parkinson induced mice model at 5 mg/kg body weight without any toxicity and recently one of the molecule has successfully cleared phase I human clinical trials.

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. M. P. P., de Sena L. S., Franco, T. L., Montagnoli, C. A. M. Fraga, *Expert Opinion on Drug Discovery*, **2024**, 19, 451.
4. A. L. Parkes, I. A. Yule, *Expert Opinion on Drug Discovery*, **2016**, 11, 665.
5. S. Manohar, D. S. Rawat, *ACS Med. Chem. Lett.* **2012**, 3, 555.
6. M. Tripathi, D. Taylor, S. I. Khan, B. L. Tekwani, P. Ponnann, T. Velpandian, U. Das, D. S. Rawat, *ACS Med. Chem. Lett.* **2019**, 10, 714.
7. W. Kim, M. Tripathi, C. Kim, S. Vardhineni, Y. Cha, S. K. Kandi, M. Feitosa, R. Kholiya, E. Sah, A. Thakur, Y. Kim, S. Ko, K. Bhatia, S. Manohar, Y.-B. Kong, G. Sindhu, Y.-S. Kim, B. Cohen, D. S. Rawat, K.-S. Kim, *Nature Communications*, **2023**, 14, 4283.
8. D. S. Rawat, Sunny Manohar, Ummadisetty Chinna Rajesh, Deepak Kumar, Anuj Thakur, Mohit Tripathi, Panyala Linga Reddy, Shamseer Kulangara Kandi, Satyapavan Vardhineni, Kwang-Soo, and Chun-Hyung Kim, Amino-quinoline based hybrids and uses thereof. Pub no: US 2017/0209441 A1; EP Application No. 13758678; PCT/US2013/28329; WO2013134047 A3, PCT/US2013/028329 (**2013**). US 11,026,943 B2 (**2021**).

DEVELOPMENT AND ASSESSMENT OF CUBOSOMAL NANO FORMULATION LOADED WITH BETA-SITOSTEROL FOR IMPROVING OF ANTIOXIDANT ACTIVITY

Disha Dutta, Ramsha Aslam, Vikas Bhatt, Priya Pandey
Devsthal Vidyapeeth College of Pharmacy, Lalpur, Rudrapur

The limitations of synthetic drugs, which are commonly characterized by limited bioavailability and poor water solubility, make treating dermatological conditions difficult. According to recent research, beta sitosterol (β -ST), a naturally occurring substance known for its strong anti-inflammatory and antioxidant qualities, may be used as a treatment for conditions affecting the skin. This study explores the encapsulation of beta sitosterol within cubosomal nano-formulations as a solution to the problems of bioavailability and solubility related to hydrophobic bioactives. Glyceryl monooleate (GMO) and Poloxamer 407 (P407) were used as the lipid phase and polyvinyl alcohol (PVA) as the aqueous phase in the emulsification process utilized to create cubosomes. The physicochemical characteristics of the cubosomes loaded with β -ST were thoroughly examined. Particle size, zeta potential, scanning electron microscopy (SEM), encapsulation efficiency, and differential scanning calorimetry (DSC) evaluations were all part of the characterization process. A uniform distribution was suggested by the experimental data, which showed an average particle size of 139.7 nm, a zeta potential of -15.17 mV, and a low polydispersity index of 0.225. SEM imaging verified the improved formulation's cubic structure and nanoscale dimensions. The formulation also showed a positive yield and great encapsulation efficiency. Ascorbic acid was used as a comparison standard in the DPPH experiment to evaluate the antioxidant activity of the β -ST-loaded cubosomes. According to the study's findings, cubosomal encapsulation offers a viable method to improve antioxidant activity, and facilitating regulated medication release—all of which eventually contribute to long-term storage stability.

Keywords: β - Sitosterol, Cubosomes, Nano formulation, Skin disease, Topical delivery

DEVELOPMENT OF ALLOSTERIC INHIBITORS AGAINST CYCLIN-DEPENDENT KINASE 2 (CDK2)

Gunda I. Georg

University of Minnesota

Cdk2 has been genetically validated as an anti-cancer and male contraceptive target. Transgenic mice overexpressing cyclin E are resistant to breast cancer carcinogenesis when Cdk2 is genetically knocked out. Additionally, Cdk2 is a dispensable protein for healthy cells; Cdk2 knock-out mice are viable, but male mice are infertile. This implies that selective inhibition of Cdk2 could be an effective and safe therapy for many patients with ovarian and other cancers and be used for reversible male contraception. The discovery and evaluation of several potent and selective allosteric CDK2 inhibitors using high throughput screening and structure-based drug design will be discussed.

PROTEIN FUNCTION & STRUCTURE: NOVEL REVELATION

Indira Ghosh

Former Professor & Dean, School of Computational & Integrative Sciences, Jawaharlal
Nehru University, New Delhi 110067

Biological Macromolecules always throw new challenges to inspire biologists to interpret their data, especially mechanistic concepts to build. With the knowledge of too many protein structures in deeper detail, protein structures are well characterized and projected as very compact in nature but functionally highly flexible. “How has this happened?”. Many answers are available, like Dynamics of protein structure, different folding with smallest change in sequence, limited secondary structures, thermodynamics of stable protein etc. As the prediction from sequence to structure is reaching a new height, thanks to AI tools, we are intrigued to learn more at the local events in protein structures, like modularity, compactness, interaction space, as these will affect our designing of small molecules to impair the activity.

We discuss here a systematic approach to identify structural modules using component-based approach by considering the arrangement of secondary structural elements (SSEs), strict geometrical sense. For concise representation of contact among SSEs in proteins, “contact string” has been developed, like “fingerprints”, which can uniquely represent all different contact patterns, which unravel all possible structures. However, it’s interesting to observe that functional proteins are very choosy, only a few patterns occur. Our group has developed ProLego, an application to explore the component aspect of protein structures and provide an intuitive and efficient way to scan the protein topology space. One interesting observation was that the set of topologies that are found to be structurally prevalent are functionally divergent. Identification of the smallest component of protein’s modular structural arrangement will provide an insight into its evolution and structural–functional space.

References:

- Khan T, Ghosh I. (2015) Modularity in protein structures: study on all-alpha proteins. *J Biomol Struct Dyn.*;33:2667–81.
- Taushif Khan, Shailesh Kumar Panday and Indira Ghosh. (2018) ProLego: tool for extracting and visualizing topological modules in protein structures. *BMC Bioinformatics* (2018) 19:167.

DRUG EFFICACY AND SEX DIFFERENCES IN IMMUNE RESPONSES

Lakshmi P. Kotra

Professor, Leslie Dan Faculty of Pharmacy, University of Toronto, and
Senior Scientist, Krembil Research Institute, University Health Network

Males and females respond differently to inflammatory insults, and it is also known that sex hormones play a role influencing inflammatory pathways. Endocannabinoid system (ECS), an integral part of inflammatory and immune responses, also behaves differently in males and females. Cannabidiol (CBD), a plant cannabinoid and antagonist to CB2 receptor in the ECS, is a popular molecule and is widely used for its anti-inflammatory properties. CBD is a bicyclic terpenoid derivative with two chiral centers. It is used widely by patients suffering from inflammatory disorders such as arthritis. We studied the anti-inflammatory activities of CBD in male and female mice using an Experimental Autoimmune Encephalomyelitis (EAE) mouse model to understand drug efficacy and sex differences. EAE was induced in C57BL/6J mice by immunization with MOG₃₅₋₅₅ peptide, and pertussis toxin. Three cohorts, healthy mice, vehicle-treated and CBD-treated male and female mice were analyzed. CBD-treated cohorts showed noticeable differences between male and female groups, and when compared to the vehicle-treated cohort. These differences are seen in the peripheral inflammatory cells, cytokines as well as infiltration of the peripheral immune cells into the brain and spinal cord. In general, male animals experienced more severe disease onset but responded better than females to the CBD treatment. CBD treated male mice had significantly lower area of inflammation in the spinal cord, fewer brain-invading T cells, and lower count of microglia/macrophages in the spinal cord. These studies suggest that endocannabinoid system and its modulation have an effect on peripheral and central immune system differentially in males and females.

REVOLUTIONIZING HEALTHCARE OPERATIONS WITH SAP: INNOVATION, INTEGRATION, AND IMPACT

Prakhar Saraswat

SCM Yuga Technologies Pvt Ltd.

In the rapidly evolving healthcare and life sciences sectors, advanced digital technologies are crucial for ensuring operational excellence, regulatory compliance, and patient-centric care. SAP Advanced Track and Trace for Pharmaceuticals (SAP ATTP) emerges as a transformative solution, enabling pharmaceutical companies to meet global serialization and traceability mandates. This robust platform facilitates end-to-end product tracking, minimizes counterfeit risks, and ensures supply chain transparency, fostering trust among stakeholders. SAP's innovative solutions extend beyond pharmaceuticals, revolutionizing healthcare operations through SAP S/4HANA and SAP Business One ERP. These platforms empower healthcare organizations to streamline processes, enhance data-driven decision-making, and optimize resource utilization. By integrating predictive analytics and real-time insights, they enable superior patient care, compliance with stringent regulatory standards, and cost efficiencies. Further advancements in life sciences and senior care are driven by SAP's commitment to innovation, as highlighted by its strategic focus on digital transformation. Solutions like SAP S/4HANA for Healthcare and SAP Business One cater to the unique needs of hospitals and care facilities, enabling improved patient engagement, operational agility, and staff productivity. The integration of these technologies' underscores SAP's pivotal role in redefining healthcare and life sciences. From secure track-and-trace systems for pharmaceuticals to transformative ERP solutions, SAP drives exceptional outcomes across industries. These innovations enhance patient safety, ensure compliance, and set new benchmarks for operational efficiency, paving the way for a smarter, more connected future in healthcare and life sciences.

NOVEL CHIRALITY DESCRIPTORS FOR THE PREDICTION PHARMACOLOGICAL AND TOXICOLOGICAL ACTIVITIES OF CHIRAL MOLECULES

Ramanathan Natarajan¹ and Subhash C. Basak²

¹Saranathan College of Engineering, Tiruchirappalli 620012, Tamil Nadu, India

²Retired Adjunct Professor, Department of Chemistry and Biochemistry and Senior Scientist,
Natural Resources' Research Institute, University of Minnesota Duluth, MN, USA

The human body contains numerous chiral macromolecules owing to the homochiral nature of the building blocks and therefore is an amazing chiral selector. Thus, the human body will interact with the enantiomers of the drug differently and metabolize each enantiomer by different pathways generating difference in the pharmacological activity. One enantiomer may produce the desired therapeutic activity, while the other may be inactive or, in the worst scenario, produce undesired effects or toxicity to nontarget tissues. This revelation had changed the strategy in the pharmaceutical industry for the manufacture of chiral drugs and resulted in the synthesis and “chiral switching” to more and more enantiopure drugs. Numerical characterization of chirality was attempted by several others to extend the QSAR approach for predicting pharmacological and toxicological effects of chiral molecules. Most of these approaches in numerical characterization of enantiomers derive only a binary set of descriptors. A single set of chiral indices that is able to model the biological response of a SINGLE target may fail to model the biological responses of a different target that is uncorrelated. Moreover, the neighbourhood of the chiral center (atom) in a molecule plays an important role in the interaction of the chiral molecule with the receptor. Hence, we need a collection of mutually different chirality indices for the QSAR of chiral molecules of different chemical classes or different bioactivities of the same set of molecules. To meet this requirement, a series of relative chirality indices (RCIs) based on the weighted graph models of the neighbourhoods of chiral centers in the molecules is developed. Application of the multidimensional space of the novel family of RCIs in the quantitative chiral structure-activity relationship (QCSAR) studies of different classes of chemicals will be presented.

Keywords: Chirality indices; QSAR; molecular descriptors; numerical characterization, enantiomers.

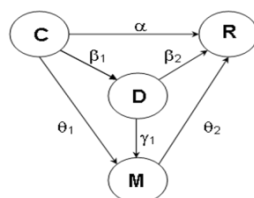
MATHEMATICAL DESCRIPTORS OF MOLECULES AND BIOMOLECULES: THEIR NATURE, DEVELOPMENT AND APPLICATIONS

*Subhash C. Basak¹, Smarajit Manna², Marjan Vracko³, Constanza Cardenas Carvajal⁴,
Tathagata Dutta⁵, Aritra Banerjee⁶, Ramanathan Natarajan⁷ and Gregory D. Grunwald⁸*

¹ Retired Adjunct Professor, Department of Chemistry and Biochemistry, University of Minnesota, Duluth, MN, USA. sbasak@d.umn.edu; ² Jagadis Bose National Science Talent Search, 1300 Rajdanga Main Road, Kolkata – 700107, India; ³ National Institute of Chemistry, Ljubljana, Slovenia; ⁴ Núcleo Biotecnología Curauma, Pontificia Universidad Católica de Valparaíso, Fono: 56322274826, Av. Universidad 330 Curauma, Valparaíso-Chile; ⁵ Center for Interdisciplinary Research & Education, Kolkata, India; ⁶ University of Minnesota Twin Cities, USA; ⁷ Saranathan College of Engineering, Tiruchirappalli, Tamil Nadu, India;

⁸ Natural Resources Research Institute, University of Minnesota Duluth, USA

Recent upsurge in the use of descriptors were fueled by (a) Development of novel concepts in the characterization of molecular structure, (b) Easy accessibility to software and high-speed computers capable of calculating relevant descriptors from structure fast (c) Availability of sufficiently large databases of experimental properties and (d) ready obtainability of statistical and machine learning methods for the development and validation of robust predictive models for basic research and their practical applications in decision support systems in current regulatory and industrial protocols for chemical evaluation. Descriptors were used in the characterization of closely related structures like isospectral graphs, quantification of similarity/ dissimilarity of chemical and biological structures, formulation of quantitative structure-activity relationship (QSAR) models and quantification of DNA/ RNA sequences as well as experimental proteomics patterns. Such wide applications of descriptors in wide areas of chemistry, drug discovery, predictive toxicology and chemobioinformatics follow from the basic philosophy of the structure-property similarity principle (SPSP) as shown in the figure below:



An empirical property is a function $\alpha: C \rightarrow R$ which maps the set C of compounds into the real line R . A non-empirical SAR may be looked upon as a composition of a description function

$\beta_1: C \rightarrow D$ mapping each chemical structure of C into a space of non-empirical structural descriptors (D) and a prediction function $\beta_2: D \rightarrow R$ which maps the descriptors into the real line. When $[\alpha(C) - \beta_2 \beta_1(C)]$ is within the range of experimental errors, we say that we have a good non-empirical predictive model.

MOLECULAR MECHANISMS OF ALLOSTERIC CHANGES IN DRUG TARGETS: INSIGHTS FROM MOLECULAR DYNAMICS AND MACHINE LEARNING

Shubhra Ghosh Dastidar

Bose Institute, EN 80, Sector V, Bidhannagar, Kolkata, India

Allosteric changes in the conformations of the biological macromolecules are of tremendous importance for their functions and existence of such mechanism in a system gives a unique opportunity to design drugs with higher precisions. This is because allosteric changes could also be induced by administering small molecules to activate a macromolecule to function or to inactivate it. While state-of-art experiments can suggest the existence of allosteric transitions in a molecular system, the mechanisms and atom-atom interaction network of allostery in a molecule are often non-trivial to understand just from the static models of molecular structures. The insights into allostery are obtainable from the computational modelling and simulations of their dynamics which can show the molecules in their action, revealing a more realistic scenario. This presentation will address this issue with examples of various molecular systems like α , β -Tubulin¹⁻⁴, Bcl2⁵, kinases⁶⁻⁷, all of which are of tremendous importance in the field of drug design to combat cancer. Not only the structural and thermodynamic insights which will be presented, but also our latest initiatives to use machine learning⁷ methods to complement the molecular dynamics simulations will be briefly discussed.

Keywords: Allostery, Kinase, Tubulin, Molecular Dynamics, Machine Learning

References:

1. Basu D, Ghosh Dastidar S, Comput Biol Chem. 2024; 108, 108004
2. Majumdar S, Basu D, Ghosh Dastidar S, J Chem Inf Model 2019; 59, 2274-2286.
3. Majumdar S, Ghosh Dastidar S, J Phys Chem B 2017; 121, 118-128.
4. Majumdar S, Maiti S, Ghosh Dastidar S, Biochemistry 2016, 55, 335-47.
5. Sinha S, Maity A, Ghosh Dastidar S, J Chem Inf Model. 2018, 58, 370-382
6. Ray Chaudhuri N, Ghosh Dastidar S, J Chem Inf Model 2023, 63, 224-239.
7. Ray Chaudhuri N, Ghosh Dastidar S, Biochemistry 2024, 63, 1474-1492

**TO EXPLORE BIOCHEMICAL MECHANISMS OF CHEMO PREVENTIVES
AGAINST COLORECTAL CANCER UTILIZING DOCKING SIMULATION***Anjali Negi and Sisir Nandi*Global Institute of Pharmaceutical Education & Research (GIPER), Kashipur-244713,
Uttarakhand, IndiaE-Mail: sisir.iicb@gmail.com

Colon is a major organ of the gastrointestinal system. There is a good friendship between colon, liver, pancreas, and lungs which are very important metabolic organs. The colon becomes under pressure due to improper intake of diet, abnormal lifestyle, lack of night sleeping, mental stress, bacterial and viral infections which cause negative environment for the microbiomes and further loss of microbiome may produce colorectal disorders like indigestion, flatulence, gastritis, irritable bowel syndrome, constipation and colon cancer due to aberrant expression of certain genes on abnormal signaling. Lactulose, vitamin A, vitamin E, vitamin C and N-acetyl cysteine (NAC) have been reported to combat the colorectal cancer. But the molecular mechanisms are yet to explore against overexpression of certain genes like KRASG₁₂C. Therefore, an attempt has been made in the present study to explore the biochemical mechanisms of Lactulose, vitamin A, vitamin E, vitamin C and N-acetyl cysteine (NAC) having affinity towards the active site of KRASG₁₂C taking docking as the molecular simulation.

WORKING IN A GOOD LABORATORY PRACTICE (GLP) ENVIRONMENT; THE POSITIVE OUTCOMES

Srikanta Kumar Rath

Toxicology & Experimental Medicine Division
CSIR- Central Drug Research Institute

Good Laboratory Practices (GLP) are guidelines that ensure the quality and integrity of data generated in the laboratory. There are several benefits to practicing it. The data generated in such an environment ensures credibility and reliability as this data is used to assess the safety of products and pass through stringent regulatory decisions to protect human health and the environment. GLP ensures animal healthcare and ethical treatment of animals. Wasteful research is also controlled and efficient data collection is in place which overall reduces the cost of research and also facilitates international acceptance. In this way it helps to build trust in the scientific process and in the products that are developed using scientific research. The data generated in the GLP environment helps to ensure that scientific findings can be reproduced anywhere in the globe and hence duplication of studies is not required which saves time. GLP helps remove technical trade barriers. Therefore, working in a GLP environment is quite distinguished and dignified. The author will share his own experience at a Test facility in the country.

MACHINE LEARNING APPLICATION FOR DETECTION OF THE POTENTIAL GEROPROTECTORS IN THE CHEMICAL-PHARMACOLOGICAL UNIVERSE

Vladimir Poroikov, Alexey Lagunin, Leonid Stolbov, Ekaterina Stolbova, Dmitry Druzhilovskiy, Dmitry Filimonov

Institute of Biomedical Chemistry, Bldg. 10/8, Pogodinskaya Str., Moscow, 119121, Russia
E-mail: vladimir.poroikov@ibmc.msk.ru

Aging is defined as a set of age-related changes in the organism, leading to a decrease in its vitality and an increase in the probability of death. Geroprotectors are the substances that slow down the aging process and prevent age-related diseases. The mechanisms of anti-aging action discussed in the literature outline criteria for *in silico* identification of potential geroprotectors among the pharmacological substances. Intersection of the terms described mechanisms of anti-aging action with the biological activities in PASS (Prediction of Activity Spectra for Substances) revealed the opportunity for development of special computational tool. The PASS GERO program predicts 115 mechanisms of geroprotective action with the average Invariant Accuracy of Prediction in leave-one-out and 20-fold cross-validation equals to 0.9665 and 0.9659, respectively; which demonstrates high accuracy and predictive ability. For validation of this computational tool, we performed the prediction of geroprotective activity profiles for 15 reference compounds. For each reference compound, a certain number of geroprotective action mechanisms are predicted in congruence with known activities. Thus, PASS GERO may be used for selection of new potential geroprotectors by virtual screening. It is reasonable to continue further improving machine learning models, both by replenishing the training sets with new information on potential geroprotectors, and taking into account the evolution of general concepts regarding geroprotection.

This research was supported by the Ministry of Science and Higher Education of the Russian Federation within the framework of Agreement No. 075-15-2024-643.

Keywords: aging, geroprotectors, *in silico* evaluation, machine learning, PASS GERO

ABSTRACTS OF ONLINE ORAL PRESENTATIONS

ADVANCES IN MICROSPONGE TECHNOLOGY FOR CONTROLLED DRUG DELIVERY: A COMPREHENSIVE REVIEW

Aayushman Singh¹, and Poonam Gangwar^{2}*

**Department of Pharmaceutics, School of pharmaceutical Sciences,
Shri Guru Ram Rai University, Patel Nagar, Dehradun*

Microsponges are polymeric microparticles with an internal porous structure capable of encapsulating various drugs. This abstract provides an overview of microsphere formulation, encompassing preparation methods, characterization techniques, and applications. The quasi-emulsion solvent diffusion method is a commonly employed technique for microsphere production, involving the formation of an oil-in-water emulsion followed by solvent evaporation. Characterization of microspheres includes particle size analysis, drug loading, encapsulation efficiency, and release kinetics. Microspheres offer advantages such as sustained drug release, improved drug solubility, and enhanced skin penetration. Potential applications span various therapeutic areas, including dermatology, ophthalmology, and oral delivery. Ongoing research focuses on optimizing microsphere formulations for specific drug molecules and therapeutic indications to achieve desired drug release profiles and efficacy. Recent advancements in microspheres have focused on enhancing their loading capacity, stability, and release profiles through the development of novel synthesis techniques, such as solvent evaporation, coacervation, and supercritical fluid processing. Furthermore, the surface modification of microspheres allows for better targeting of specific tissues or skin layers, improving the precision of drug delivery or cosmetic treatments. This review delves into the preparation methods, characterization techniques, and diverse applications of advanced microspheres. It also addresses the challenges associated with scaling up production and regulatory considerations for their widespread adoption. The future of microspheres appears promising, with ongoing research aimed at optimizing their design for personalized medicine, skincare, and more efficient therapeutic outcomes.

Key Words: microspheres, drug delivery, sustained release, quasi-emulsion solvent diffusion, characterization.

COMPARATIVE ANALYSIS OF AZELNIDIPINE CO-CRYSTAL FORMATION: SOLVENT EVAPORATION VS. WET GRINDING FOR ENHANCED SOLUBILITY

Aparna Joshi, and G. Gnana Rajan

School of Pharmaceutical Sciences SGRR University, Dehradun

Azelnidipine, a calcium channel blocker with poor aqueous solubility, faces challenges in drug formulation and bioavailability. Co-crystallization offers a promising approach to enhance its solubility and dissolution. This study compares two co-crystal formation techniques: wet grinding and solvent evaporation. Notably, the solvent evaporation method yielded well-defined, highly crystalline co-crystals visible to the naked eye, exhibiting superior stability and structural integrity. In contrast, wet grinding produced smaller co-crystals with increased surface area, leading to faster dissolution. Characterization using, DSC, FTIR, and SEM confirmed successful co-crystal formation and molecular interactions. The findings highlight solvent evaporation as a superior method for obtaining high-quality co-crystals, making it a promising approach for improving Azelnidipine pharmaceutical performance.

Keywords: Azelnidipine, co-crystals, solvent evaporation, wet grinding, solubility enhancement, crystallinity.

References:

1. Q. Lu, J. Dun, J.M. Chen, S. Liu, C.C. Sun, Improving solid-state properties of berberine chloride through forming a salt cocrystal with citric acid, *Int J Pharm* 554 (October 2018) (2019) 14–20.
2. P. Cerreia Vioglio, M.R. Chierotti, R. Gobetto, Pharmaceutical aspects of salt and cocrystal forms of APIs and characterization challenges, *Adv. Drug Deliv. Rev.* 117 (2017) 86–110.

FORMULATION AND EVALUATION OF DRUG-PHOSPHOLIPID COMPLEX FOR SOLUBILITY ENHANCEMENT

Vishal Kapoor¹, Gauree Kukreti², Archana Dhyani^{*3}, Sumit Durgapal⁴, and Alka Singh⁵

^{1,2}School of Pharmaceutical Sciences and Technology, Sardar Bhagwan Singh University, Balawala, Dehradun 248161, Uttarakhand, India.

³School of Pharmacy, Graphic Era Hill University, Clement town, Dehradun, 248001, Uttarakhand, India.

⁴Department of Pharmaceutics, Uttarakhand Institute of Pharmaceutical Sciences, Uttarakhand University, Premnagar, Dehradun, 248007, Uttarakhand, India

⁵ School of Pharmaceutical Sciences and Technology, Sardar Bhagwan Singh University, Balawala, Dehradun 248161, Uttarakhand, India.

The research work mainly aimed at the formulation development and *in-vitro* evaluation of cilnidipine phospholipid complex and matrix dispersion. Cilnidipine is a BCS class II drug that is having low solubility and high permeability. The drug is generally used as antihypertensive agent. The main problem with the drug is its low bioavailability which is due to the low solubility of the cilnidipine in aqueous medium. In the present investigation, egg lecithin was used as a phospholipid and drug-phospholipid complex was prepared by solvent evaporation method which was further formulated to matrix dispersion. Cilnidipine and phospholipid were taken in different molar ratios by varying the temperature and time keeping the rpm constant. The solvent was evaporated through rota evaporator. Due to the stickiness in the prepared drug-phospholipid complex, it was further formulated to prepare matrix dispersion by the addition of PVA as a polymer which increases the dispersibility of the drug. Formulated drug-phospholipid complex and matrix dispersion were subjected to various characterization that are percentage yield, entrapment efficiency, solubility, FTIR, DSC, PDI, zeta potential and *in vitro* drug release studies. The optimized formulation 1 was selected and used for the preparation of matrix dispersion. From the above results it can be concluded that the prepared drug-phospholipid complex and matrix dispersion showed a 2-fold increase in the drug release when compared with the pure drug cilnidipine.

Keywords: Bioavailability, phospholipid complex, solubility, dispersion.

COMPARISON OF 2D AND 3D CANCER CELL CULTURES: DIFFERENT TYPES AND THEIR CHARACTERISTICS

Asha Gummadi¹, and Ramaniaha Gangireddy²

Department of Pharmacology, K V S R Siddhartha college of pharmacy, Vijayawada- Andhra Pradesh, India

Cell culture is a widely used in vitro tool for advancing our understanding of cell biology, tissue morphology, disease mechanisms, drug action, protein production, and tissue engineering. Most cancer biology research relies on two-dimensional (2D) cell cultures in vitro. However, 2D cultures have several limitations, including disrupted interactions between cells and their extracellular environment, altered cell morphology, polarity, and division methods. These drawbacks have driven the development of models that better mimic in vivo conditions, such as three-dimensional (3D) cultures. Optimizing culture conditions can enhance our understanding of cancer biology and facilitate biomarker studies and targeted therapies. This review compares 2D and 3D in vitro cultures, along with different types of 3D culture models.

Keywords: co-culture, cell culture methods, 3D culture, 2D culture, cancer research.

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL SCREENING OF NOVEL HETEROCYCLIC -2-OXO-2H-CHROMENE-3-CARBONYL) SPIRO[INDOLINE-3,3'-PYRAZOLIDIN]-2-ONE BASED DERIVATIVES

Tandrani Ghosh¹, **Geet Gupta**², Vaishnavi Dwivedi¹, Nitin Srivastava^{2*}, and Krishna Srivastava^{1*}

¹Faculty of Chemical Sciences, SRM University Lucknow-Dewa Road, Barabanki- 225 003, India

²Department of Chemistry, Amity University Uttar Pradesh, Lucknow Campus-226028, India

A series of novel pyrazole-spiro based cyclized derivatives of acetyl, iminoethyl and ethanethioyl were synthesized and screened for antimicrobial activities. The final derivatives were procured by initiating the condensation of precursor molecules, salicylaldehyde and ethyl acetoacetate form acetyl coumarin. The obtained products were allowed to react with substituted-isatin which then yielded chalcone. Upon further reaction of chalcone with hydrazine hydrate, aminoguanidine HCl and thiosemicarbazide we got final products as 1'-acetyl-5- substituted -5'-(2-oxo-2H-chromene-3-carbonyl)spiro[indoline-3,3'-pyrazolidin]-2-one (**3a-c**), 5- substituted -1'-(1-iminoethyl)-5'-(2-oxo-2H-chromene-3-carbonyl)spiro[indoline-3,3'-pyrazolidin]-2-one (**4a-c**) and 5- substituted -1'-ethanethioyl-5'-(2-oxo-2H-chromene-3-carbonyl)spiro[indoline-3,3'-pyrazolidin]-2-one (**5a-c**). The structures of all synthesized derivatives were identified by their spectral data. The synthesized compounds exhibited promising *in-vitro* antimicrobial activity against Gram-positive bacteria (*S. Aureus*, *B. subtilis*), Gram-negative bacteria (*Klebsiella pneumoniae*), and Fungi (*Candida albicans*) as compared to the standard drug Chloramphenicol and Ketoconazole.

Keywords: Isatin, thiourea, salicylaldehyde, 1,4-dioxane, semicarbazide, hydrazine hydrate, antimicrobial activity.

SYNERGISTIC ANTIFUNGAL ACTIVITY OF FLUCONAZOLE EMULGEL CONTAINING VARIOUS OILS

***Heena Farooqui**^{1*}, Mohd. Vaseem Fateh² and Sarfaraz Ahmed¹*

¹Global Institute of Pharmaceutical Education and Research, Kashipur, Uttarakhand, 244713;

²Burman Group of Institutions Roorkee Haridwar Uttarakhand 247667.

This study focuses on the Fluconazole-based solid dispersion incorporated into emulgels with natural oils for antifungal synergistic effect agents like Lemongrass oil, Neem oil, Tulsi oil. Due to fluconazole's low aqueous solubility, solid dispersion formulations were prepared with β -cyclodextrin and PVP as carriers. Among six formulations, F2 was identified as the most effective, demonstrating the highest aqueous solubility (78.41%), drug content (98.68%), and dissolution rate (99.23%). The results indicate that EGF2 has a stronger inhibitory effect on the tested microorganisms compared to Fluconazole gel (1g). *Candida albicans*: EGF2 exhibited a significantly larger zone of inhibition (27.7 ± 1.7 mm) compared to Fluconazole gel (19.9 ± 3.5 mm), highlighting EGF2's superior antifungal activity against this common pathogen. *Candida esophagitis*: Similar trends were observed for *Candida esophagitis*, with EGF2 showing a zone of inhibition of 26.7 ± 2.2 mm, while Fluconazole gel displayed 18.5 ± 0.9 mm. Furthermore, EGF2 showed substantially higher retention on the SC layer (569.62 ± 12.45 $\mu\text{g}/\text{cm}^2$) compared to the marketed formulation (327.15 ± 19.06 $\mu\text{g}/\text{cm}^2$). This higher retention suggests superior adhesive properties or better penetration of EGF2, ensuring more of the active ingredient remains in the skin. The Emulgels also demonstrated reasonable stability in terms of drug content analysis and physicochemical characteristics, making them a promising option for antifungal treatments.

Keywords: Gel, Lemongrass, Neem, Emulgel, Antifungal

FORMULATION AND EVALUATION OF METHYL METHACRYLATE GRAFTED COPOLYMER OF NEEM GUM BY GRAFTING TECHNIQUE

Neetu Rajpoot, and Dinesh Puri*

School of Pharmacy, Graphic Era Hill University, Dehradun, Uttarakhand

The use of natural polymers as drug delivery and trapping vehicles has become widespread. Natural polymers exhibit greater biocompatibility, biodegradability, and ease of accessibility as compared to synthetic polymers. Additionally, the native natural polymers reactive groups allow for interaction with other functional groups. Such alteration changes the physical and chemical properties of the newly formed polymer and gives it remarkable functions. Neem gum is a transparent, vivid, amber-colored substance that dissolves in cold water and has no harsh taste. It is employed in the production of special purpose foods and as a bulking agent. Neem gum is used in pharmaceuticals as a film coating, thickening agent, slow-release agent, and tablet binder. Additionally, it can be used to improve solubility. In the present study, we aimed to develop grafted copolymer of neem gum (PMMA-g-NG) via grafting neem gum (NG) with methyl methacrylate (MMA) chains by using microwave assisted grafting technique. The free radical induced grafting method was adopted to graft neem gum with methyl methacrylate, using ceric ammonium nitrate (CAN) as a redox initiator. The impact on grafting parameters such as grafting percentage and grafting efficiency (GE), of monomer and initiator concentrations was evaluated. FTIR study proved the grafting phenomenon and PMMA-g-NG showed significant swelling and water retention capacity. The batch with higher grafting efficiency and percentage grafting was selected and characterized by DSC, FT-IR spectroscopy.

Keywords: Biocompatibility, Efficiency, Grafting, Microwave, Thickening.

PROGRESSIVE LIPID-BASED NANOCARRIERS TO TREAT NEUROLOGICAL DISORDER

Nirvesh Chaudhri, Vaibhav Rastogi*

TMU- Teerthankar Mahaveer University, College of Pharmacy, Moradabad,
244001. India

The recently developed novel nano-techniques have been employed for the sustainable treatment of various diseases like Neurological disorders including Alzheimer's, Parkinson's, Schizophrenia, multiple sclerosis, neuro infections, epilepsy, and malnutrition. The cerebrospinal fluid barrier and other blood-brain barriers defend the Central nervous system from drug particles reaching the brain's intended region. These problems are treated with advanced forms of nanocarriers. The “lipid based Nanocarriers” offer unique benefits compared to other carriers like micelles, liposomes, nanoparticles, etc. Due to their compatibility with the BBB layer, the nano-sized lipid-based carriers system is the ideal solution for medication delivery to the central nervous system. The easy incorporation of drug molecules into neuronal cells, results in enhanced stability and greater concentration. The “lipid-based nanocarriers” are fabricated with various techniques like “high-speed homogenization”, sonication, solvent evaporation, and emulsification methods. In this formulation, solid lipids, liquid lipids, and polymers regulate drug transport to the brain and enhance therapeutic potential in neurological treatment. This approach improves therapeutic outcomes by enabling safe and effective targeting in chronic neurological disease treatment. In this study, we delve into the current advancements in nanotechnology for neurological therapy and elucidate their mechanisms of action.

Keywords: Nanotechnology, Lipid Nanocarriers, Neurological disease, Drug delivery.

GREENER SYNTHESIS OF QUINOLINES USING IONIC LIQUIDS

Nitin Srivastava

Department of Chemistry, Amity university Uttar Pradesh Lucknow Campus-226028

Quinoline moiety is a fundamental core in the large number of natural compounds and pharmacologically active substances, which are significant in pharmaceuticals. They have exhibited their potential antiviral, antibacterial, antimalarial, antitubercular, anti-HIV, anticancer, compounds with a quinoline motif demonstrate a variety of biological and pharmacological analgesic, anti-inflammatory, antihypertensive, anti-Alzheimer etc. They have also been employed as fluorescent probes in the diagnosis of various ailments. There are many quinoline based drugs like quinine, quinidine, chloroquine, and mefloquine which are being marketed. Ciprofloxacin and Sparfloxacin are quinoline-based antimicrobial drugs; Camptothecin and Irinotecan are anticancer drugs; Saquinavir and Vesnarinone (cardiotonic) are HIV-1 protease enzyme; Bedaquiline is a quinoline-based antimycobacterial drug. Sustainable development demands cleaner greener synthesis in the pharmaceutical sector. Cleaner, greener synthesis may be done with the help of ionic liquids which are versatile class of green solvents which have several advantages over traditional medium. Ionic liquids are “designer solvents” whose properties like solubility, density, refractive index, and viscosity can be ameliorated to fit better as per requirements. This is done by structural modification of its anionic or cationic part or both. Ionic liquids have been extensively employed for the several synthetic transformations desired in medicinal chemistry. Heterocycles, which possess key roles in medicinal chemistry, have been synthesized using a variety of structurally diverse ionic liquids. Among these heterocycles quinoline possesses a prominent role in drug discovery research and its cleaner greener and efficient synthesis need to be explored *via* ionic liquids. In this review, the recent advances in the synthesis of various kinds of quinolines using a variety of ionic liquids has been reviewed to give an overview of the cleaner, greener and sustainable synthesis of quinolines using ionic liquids.

Keywords: Heterocycles, quinolines, Ionic liquids, Drug development, medicinal chemistry

DOCKING BASED SCREENING OF POTENT NATURAL COMPONENTS TO COMBAT COVID-19-ASSOCIATED BRAIN FOG

*Sisir Nandi¹, Rachana Belwal¹, **Rishita Dey²**, and Asmita Samadder²*

¹Global Institute of Pharmaceutical Education and Research (Affiliated to Veer Madho Singh Bhandari Uttarakhand Technical University), Kashipur-244713, India.

²Cytogenetics and Molecular Biology Lab., Department of Zoology, University of Kalyani, Kalyani, Nadia, 741235, India

COVID-19 is an infectious disease caused by a novel corona virus SARS-CoV-2 strain (nCoV) and has become a deleterious issue around the globe since December 2019, prominently from Wuhan, China. Millions of lives were destroyed hampering the economy and social security. Even WHO declared as dreadful pandemic disease that negatively impacted human unity and pressurized the brain to be bound under isolation. SARS-CoV-2 damages the lungs, heart, forced liver and even neuronal vascular endothelium, resulting in brain fog, lethargy and tremors. Although COVID-19 can cause a variety of extrapulmonary symptoms, the heart, brain, and kidneys are especially vulnerable. This vascular component of COVID-19 may contribute to the explanation of the brain fog that some people experience a few months after the virus has cleared. The global COVID-19 pandemic has baffled several scientists and researchers with its versatile consequences and behavior in the etiology of several diseased conditions in post-COVID patients. The indirect and direct negative impact of COVID-19 on memory and other cognitive brain fog in humans is now a major research arena in almost all countries. There hardly exists any allopathic medicine for the treatment of COVID-19-associated brain fog. The current investigation aims to investigate the pathophysiology of the disease and structure-based screening of natural compounds to combat the dreadful post-COVID symptoms of brain fog due to neuro-inflammation followed by degeneration. Thus, a person detected with SARS-CoV-2 infection can be dealt with naturopathy to help in the recovery of memory-loss-function and combat associated neurological complications.

ABSTRACTS OF OFFLINE POSTERS

**UNDERSTANDING THE MEDICINAL AND THERAPEUTIC POTENTIAL OF
ALKALOID-BASED PHYTOCOMPOUNDS FOR THE TREATMENT OF
ALZHEIMER'S DISEASE**

Arnob Chakrovorty¹, Banani Bhattacharjee¹, Asmita Samadder^{1,} and Sisir Nandi^{2,*}*

¹Cytogenetics and Molecular Biology Lab., Department of Zoology, University of Kalyani,
Kalyani, Nadia, 741235, West Bengal, India

²Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and
Research (GIPER) (Affiliated to Veer Madho Singh Bhandari Uttarakhand Technical
University), Kashipur-244713, Uttarakhand, India.

Alzheimer's disease (AD) is a neurocognitive disorder that affects the central nervous system leading to dementia-like cognitive defects, effecting regular life of the individual. AD is a global problem that demands immediate medical attention. Alkaloid-based phytocompounds (ABP) hold enormous biological activity and therapeutic potential that can be utilized for treatment against AD. ABP administration in streptozotocin-induced AD model was found to improve biochemical parameters of the brain and provide neuroprotection by modulating key proteins. ABP improved brain glucose metabolism, reduced reactive oxygen species in brain tissue and improved the tissue architecture of the cortex and the hippocampus of the brain.

Keywords: Alzheimer's disease, neurodegenerative disease, phytotherapy, Swiss albino mice.

BIMP: UNVEILING THE PHYTOCHEMICAL RICHNESS OF INDIAN MEDICINAL PLANTS AS POTENTIAL THERAPEUTIC AGENTS

Dheeraj Kumar Chaurasia^{1,2}, and B. Jayaram²

¹ School of Interdisciplinary Research, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

² Supercomputing Facility for Bioinformatics and Computational Biology, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

The historical importance of Indian medicinal plants is well documented in traditional systems of medicine such as Ayurveda and Unani. These plants are renowned for their medicinal effects that enhance general well-being. With modern scientific progresses, there has been an increased interest in exploring the bioactivity of these plants to uncover the active compounds responsible for their pharmacological effects. This has given rise to a growing field of research focused on Indian medicinal plants, which extends beyond traditional practices to contemporary pharmaceutical breakthroughs. In this context, a manually curated database called BIMP is introduced here. This database provides information on 105,909 Phytochemicals found in 6,209 Indian medicinal plants. It includes information on both known and predicted targets for the compounds, along with specifics on the diseases and the target genes/proteins with information of organisms. Additionally, the database assesses physicochemical properties and drug similarity using cheminformatics tools, aiding drug discovery efforts. Of the 105,909 Phytochemicals, 72,318 comply with at least one of the major drug-likeness rules. The BIMP database represents a significant advancement in facilitating *in-silico* drug discovery processes by providing a comprehensive platform for discovering the therapeutic potential of Indian medicinal plant components. It also offers a protocol for identifying targets and molecules, streamlining the drug discovery process. It is openly accessible and offers researchers a valuable database for advancing drug development based on natural products. Database URL: <https://scfbio.iitd.ac.in/bimp>

Keywords: Indian medicinal plants, BIMP, Phytochemicals, Bioactivity, Therapeutics.

RATIONALE OF ANTIFUNAGAL AND ANTI BACTERIAL INTERVENTIONS OF IMIDAZOLE DERIVATIVES

*Divya Negi^{*1,2}, Akhilesh kumar Mishra¹, and Narendra Kumar Singh³*

¹School of Pharmacy, Babu Banarsi Das University, Lucknow, Uttar Pradesh, India-226028

²Faculty of Pharmaceutical Sciences, Amrapali University, Lamachaur, Haldwani, Nainital, Uttarakhand, India-263139

³Apex Institute of Pharmacy, Chunar, Mirzapur, Uttar Pradesh, India-231304.

Imidazole is a five-member heterocyclic molecule with two nitrogen atoms at positions 1 and 3 in the aromatic ring. It is categorized as a diazole. Clinical trials have utilized a variety of imidazole-based drugs for antifungal, antibacterial, anticancer, antiparasitic, antihypertensive, and anti-inflammatory properties. A remarkable class of chemicals with antimicrobial properties, including potent antifungal and antibacterial agents, are imidazole derivatives, which contain the imidazole ring. The biological, and therapeutic use of compounds containing imidazoles are the main topics of this review. Numerous studies have investigated the antifungal activity of imidazole derivatives, which interfere with the growth of cell membranes and the integrity of the walls of fungal cells. Likewise, their antibacterial properties have been noted in a variety of Gram-positive and Gram-negative bacteria, and they are linked to mechanisms such the suppression of nucleic acid replication, protein synthesis, and cell wall formation. We also investigate the structure-activity relationships of imidazole derivatives, focusing on their pharmacokinetic, toxicological, and biological activities. In addition to increasing the number of effective medications available to treat bacterial and fungal diseases, the discovery of new imidazole-based treatments could contribute to combating the growing threat of drug resistance.

Key words: Imidazole, antifungal, antimicrobial.

INNOVATION IN TASTE-MASKING TECHNOLOGIES: ADVANCING PEDIATRIC DRUG FORMULATIONS

Divyanshu, Mohammad Aadil, Raja Babu

Global Institute of Pharmaceutical Education & Research (GIPER)

Kashipur-244713, Uttarakhand, India

Pediatric drug compliance remains a significant challenge in pharmaceutical development, primarily due to the unpleasant taste of active pharmaceutical ingredients (APIs). This study investigates novel taste-masking techniques for developing palatable pediatric formulations. We explored a combination of microencapsulation using Eudragit E100 and cyclodextrin complexation to mask the bitter taste of a model drug, Amoxicillin trihydrate. The taste-masked microspheres were prepared using spray-drying technology and characterized through particle size analysis, encapsulation efficiency, and in vitro dissolution studies. The taste-masking efficiency was evaluated using an electronic tongue and human taste panels. Results demonstrated that the optimized formulation achieved 95% drug encapsulation with a mean particle size of $150 \pm 15 \mu\text{m}$. The electronic tongue analysis showed significant reduction in bitterness intensity ($p < 0.05$), correlating well with human panel evaluations. Drug release studies indicated minimal drug release ($< 10\%$) at salivary pH 6.8, while ensuring complete release ($> 90\%$) at gastric pH 1.2 within 45 minutes. Stability studies confirmed the physical and chemical stability of the formulation over six months. This innovative approach offers a promising solution for improving pediatric medication compliance through effective taste-masking while maintaining therapeutic efficacy.

WOUND HEALING: AN IN-DEPTH REVIEW

Fiza, Srishthi Gaur, Shahjad, Arun Kumar*

Global Institute of Pharmaceutical Education & Research (GIPER)

Kashipur-244713, Uttarakhand, India

Wound healing is a complex and intricate biological process that plays a fundamental role in the maintenance of tissue integrity and the restoration of homeostasis following injuries or surgical procedures. Understanding the mechanisms and factors that govern wound healing is not only crucial for medical professionals but also holds significant implications for patients' overall health and quality of life. This review aims to provide a comprehensive overview of the background and significance of wound healing, shedding light on the various stages of the process and the intricate interplay of cellular and molecular events that underlie it. Wound healing is not a mere localized response to injury; it represents a dynamic and highly regulated cascade of events that involve numerous cell types, signaling pathways, and extracellular matrix components. Furthermore, impaired or delayed wound healing can lead to a range of complications, including chronic wounds, infections, and excessive scarring, all of which can have profound implications for patient outcomes. Exploring the basic biology of wound healing, delving into the stages such as hemostasis, inflammation, proliferation, and remodeling. Each stage examined in detail, the specific cell types and molecular signals that drive the healing process forward. The factors that can influence and potentially hinder wound healing, from systemic conditions like diabetes to local factors such as tissue ischemia and the significance of advanced wound care techniques and therapeutic interventions, including the use of growth factors, tissue engineering, and regenerative medicine, which have the potential to revolutionize wound healing and enhance patient outcomes. This study is essential for healthcare professionals, researchers, and anyone interested in improving the quality of care for patients with wounds.

AN OVERVIEW OF MOOD DISORDER WITH A FOCUS ON DEPRESSION RELATED TO VEDIC PLANTS

Harsh Sharda, Deepak Teotia, Arun Kumar, Muneer Alam

Global Institute of Pharmaceutical Education & Research (GIPER)

Kashipur-244713, Uttarakhand, India

Ayurveda places great emphasis on maintaining positive mental well-being. Anything that disrupts the equilibrium of body and mind is recognized to cause a disease. Emotions are fundamental feelings experienced by humans. Each of us has experienced feelings of unhappiness, sadness, or discouragement at various points in our lives. However, when someone experiences feelings of anxiety, hopelessness, helplessness, worthlessness, guilt, irritability, pain, or restlessness, they fall into the classification of depression. Vishada and Avasada are two states resembling depression in Ayurveda. Vishada is characterized by a continual feeling of sadness, a sense of inadequacy stemming from fear of failure, which leads to an inability of both mind and body to operate effectively. Charaka references Vishado Rogavardhananam Agrya, indicating that Vishada is the primary element that exacerbates the disease state. Depression and other mood disorders are particularly severe as they often emerge in early life, are challenging to identify in adolescents, can be mistaken for typical behavioral variations, substance abuse, or other mental health conditions linked with elevated suicide risk. Consequently, treatment is usually commenced quite late and necessitates extended follow-up and prolonged management. Considering the facts presented in this article, we aim to provide a concise overview of the pathophysiology of depression and outline an extensive Ayurvedic strategy to address depression and related mood disorders. It also emphasizes the concealed idea of Ayurvedic psychology that can be applied in medicine to treat depression and enhance mental health.

IN SILICO EXPLORATION OF THE ANTIDIABETIC CAPABILITIES OF THE ESSENTIAL MEDICINAL PLANT EUPHORBIA

Mahvish Jamal and Mhaveer Singh

School of Pharmaceutical Sciences, IFTM University, Moradabad-244102

Diabetes mellitus (DM) is a significant metabolic disorder, currently affecting about 2.8% of the global population with metabolic diseases, and this number is projected to increase to 4.4% by 2030. The market offers various categories of drugs for DM, including sulfonylureas, biguanides, α -glucosidase inhibitors, thiazolidinediones, and non-sulfonylurea secretagogues. These drugs function by improving insulin sensitivity and secretion, complementing insulin, and stimulating glucose uptake. However, they are often associated with side effects such as hepatic failure, weight gain, tachycardia, and hypothyroidism. Herbal drugs have been used to treat various diseases, including DM. Herbal drugs are generally considered safer, more readily available, have fewer side effects, and are more economical than synthetic drugs. Euphorbia, a significant medicinal plant in the dicotyledon category, contains phytoconstituents such as flavonoids, terpenoids, and tannins, which are used to treat viral infections, rhinitis, spasms, asthma, skin diseases, and more. This plant has demonstrated in vivo antidiabetic properties, but the exact mechanisms of its phytoconstituents remain unclear and are subject to ongoing research. To investigate these mechanisms, docking studies were performed on the 3D structures of four proteins involved in type-2 DM: protein-tyrosine phosphatase 1B, α -glucosidase, and α -amylase, using 25 known phytoconstituents from the Euphorbia plant. The study's conclusions are based on docking energies and key amino acid interactions, providing insights into the possible mechanisms of the phytoconstituents.

Keywords: Diabetes mellitus, Euphorbiaceae, flavonoids, tannins, docking.

A REVIEW ON NOVEL DRUG DELIVERY APPROACH: THE TRANSDERMAL DRUG PATCHES

Meenakshi^{1}, and Charu Saxena²*

^{1*}Research Scholar, Faculty of Pharmacy, Swami Vivekanand Subharti University Meerut

²Associate Professor, Faculty of Pharmacy, Department of Pharmaceutics, Swami Vivekanand Subharti University Meerut

Currently, we take about 70% of our prescriptions orally, although their effectiveness is frequently lower than expected. A surface that is easily accessible for administering medications is the human skin. About one-third of the blood in the body circulates through the skin of the average adult, which has a surface area of about two square meters. Developing regulated medication delivery systems has been the pharmaceutical industry's main focus over the last few decades. There are around 200–250 sweat ducts and 10–70 hair follicles per square centimeter of human skin. Because it enables a gradual release of the medicine over time, the transdermal drug delivery system (TDDS) is different from other methods of administering medications to the skin. This decreases the negative effects that are typical with oral drugs and weakens the effect. To transport active substances straight into the bloodstream through the skin, designers create a variety of transdermal patches. Because they are non-invasive, eliminate the need for professional medicine administration, lessen negative effects on the gastrointestinal (GI) system, and encourage patient adherence, transdermal drug delivery (TDDS) systems are considered patient-friendly. Transdermal medication delivery does have many drawbacks, though, including the potential for skin irritation or sensitization, adhesive discomfort, poor skin adherence, high cost, and limited use of certain physicochemical drug features. The several facets of TDDS and new developments in this class of targeted therapeutic formulation in relation to acute and chronic metabolic disorders are included in our current review.

Keywords: Drug delivery, adhesive discomfort, targeted therapeutic, regulated medication, and TDDS,

THE EXOSOME EXPEDITION: NAVIGATING THE FRONTIERS OF WOUND HEALING WITH GROUNDBREAKING STUDIES, MOLECULAR MYSTERIES, AND THERAPEUTIC INNOVATIONS

Mehreen Jahan, Nishi Rani, Shahjad, and Arun Kumar

Global Institute of Pharmaceutical Education and Research, Kashipur-244713, India

Difficulties in wound healing pose a considerable clinical problem and are a significant source of morbidity in the general population. It is difficult to impossible to perform sequential studies on the same human wound, and often there are no uniform criteria for defining stages of healing or outcome of the repair process. Animal models have provided some valuable information, but the healing process differs in humans and animals, and data obtained from in vitro studies can be difficult to extrapolate to a clinical context. A clearer knowledge of what variables should be measured and what methods are best to measure them would increase opportunities for successful clinical studies. This review aims to address this need, to serve as a roadmap for both current and future researchers in the field of wound healing. Much of our knowledge of the finer details of wound healing has been elucidated through molecular and cell biology, in which the tools of genetic manipulation and cell culture studies have been invaluable. Briefly, this essay intends to synthesize our present knowledge of the processes of inflammation, epithelialization, and tissue repair primarily using evidence obtained from in vitro and in vivo studies. The basic processes involved in healing include inflammation, re-epithelialization, granulation tissue formation, and collagen remodeling. Wound healing aims to reconstruct and preserve the function of the tissue as quickly as possible. However, healing is influenced by many factors including the health and age of the individual, type, size, and site of the wound, and treatment of the wound. As a result, any deviation from the normal sequence and time course of events may result in abnormal healing. This is a vital process that all living organisms undergo at some stage in their lives. Wound healing is often divided into three or four overlapping phases.

PREDICTION OF SQUARAMIDES DERIVATIVES AS EXTERNAL DATA SET USING VALIDATED QSAR FOR THE DESIGN OF POTENT ANTI-TUBERCULAR COMPOUNDS

Muneer Alam^{1,2}, Zeeshan Fatima¹, Sisir Nandi² and Sarfaraz Ahmed²

¹Amity Institute of Pharmacy, Lucknow, Amity University Uttar Pradesh, Sector 125, Noida-201313, India

²Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research, Kashipur-244713, India.

Tuberculosis (TB) is the most important global infectious killer disease responsible for 1.8 million deaths inclusive of 0.25 million cases of drug resistance TB per year. It has emerged as a world-wide health risk due to drastic death rise in the incidence of multi drug-resistant (MDR) (rifampicin and isoniazid) and extensively drug resistant (XDR) (Fluoroquinolone and at least one of three injectable second line drugs) mycobacterial strains. Among several antitubercular drugs in clinical trials, the bedaquiline (trade name sirturo, code name: TMC207 and R207910) has emerged as a highly promising first drug approved by FDA for the treatment of multi-drug-resistant TB in combination with other drugs. Bedaquiline acts on mycobacterial ATP synthase and is highly effective on replicating as well as on dormant mycobacteria. In view of it several series of squaramides have been synthesized and evaluated for their antitubercular and ATP synthase inhibitory activities. In order to understand the role of physicochemical like hydrophobicity, electronic and steric factors in eliciting the biological response, the Quantitative structure activity relationship (QSAR) developed on Quinolines. It was observed that hydrophobic and steric parameters are more important for explaining the variations in antitubercular activity. Thus validated QSAR was taken as standard model. External data set based on Squaramides compounds have been predicted then it has been shown that some of squaramides have good predicted activity, so some of new chemical entities have been synthesized and biological activity will be carried out against tuberculosis.

DOCKING BASED QSAR STUDIES ON DHFR INHIBITORS FOR THE IDENTIFICATION OF ANTI-MALARIAL AGENTS

Nishu and Sarfaraz Ahmed

Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research, Jaspur Road, Kashipur, Uttarakhand

Malaria is a serious infectious disease caused by Plasmodium parasites, which are transmitted to humans through the bites of infected female Anopheles mosquitoes. According to the World Health Organization's (WHO) World Malaria Report 2024, there were an estimated 263 million cases and 597,000 malaria-related deaths worldwide in 2023. Hence, the continued presence of malaria on the global health agenda makes it imperative to actively seek new antimalarial agents which lead us to Dihydrofolate reductase (DHFR) which is a key enzyme in the folate pathway of Plasmodium species and offers a well-characterized antimalarial enzyme target for drug action. Docking-based Quantitative Structure-Activity Relationship (QSAR) studies provide a powerful avenue for the identification and optimization of DHFR inhibitors. This study introduces integration of molecular docking and QSAR aimed at predicting the binding affinity and biological activity of prospective DHFR inhibitors. Through the investigation of a dataset of known inhibitors, we derived QSAR models which can be used in predicting of NCE's.

**PREDICTION OF CUMULATIVE AFFINITY AND MOLECULAR MECHANISMS
OF H1 ANTIHISTAMINICS TOWARDS H1R UTILIZING STRUCTURE-BASED
DOCKING**

Sandhya Dharkiya¹, Arnob Chakrovorty², Asmita Samadder², Deepak Teotia¹ and Sisir Nandi¹

¹Global Institute of Pharmaceutical Education & Research (GIPER)
Kashipur-244713, Uttarakhand, India

²Cytogenetics and Molecular Biology Lab., Department of Zoology, University of Kalyani,
Kalyani, Nadia, 741235, West Bengal, India

Histamine is a biological amine which is released on stimulation of antigen-antibody immunological reactions. Histamine can occupy the H1 histamine receptor (H1R) and produces biological actions like triple responses of flush, flare and wheel. It causes itching, redness with inflammation followed by urticaria. Chronic urticaria is a big issue now a day. The H1 antihistaminics are given for the treatment which can occupy by H1R and antagonise the action of histamine. The molecular mechanisms are yet to explore. Therefore it is our target in the present study to explore the molecular mechanisms of a number of antihistaminic drugs utilizing structure based docking simulation. The affinity and mode of binding of the H1 antihistaminic ligands have been predicted and compared with the standard mepyramine which was co-crystallized with the active cavity of the target. The common amino acids can be taken as parameters for further H1 antihistaminic drug design.

**QUANTITATIVE STRUCTURE PHARMACOPHORE – ACTIVITY
RELATIONSHIP OF TRICYCLIC ANTIDEPRESSANTS (TCAs) UTILIZING
DISTANCE – BASED FEATURES**

Sisir Nandi, Sandhya Dharkiya, Rukayya, Shuaib Hussain, and Ankita Sharma

Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur-244713,
India.

Depression is a mental disorder which affects mood and pleasure and it is also affected by social, biological and psychological. Diagnosis and treatment of depression can improve the lives of sad people and their families and make them happier and more productive. As the COVID-19 pandemic significantly increased the incidence and prevalence of anxiety and depression across the country, there are significantly increased prescriptions of these medications perioperatively. The current study aims is to develop QSAR and pharmacophore models based on compounds pharmacophoric distances, calculated using pharmacophoric features. In the present study, 36 Tricyclic antidepressant (TCA) compounds showing antidepressant activities were gathered from the published literature. Quantitative structure pharmacophore-activity relationship (QSPAR) was developed by taking calculated pharmacophoric distances and biological activity. Developed Triangular topograph ΔABD (distance based) has shown significant distance based pharmacophore model responsible for antidepressant activities. The significant regression coefficient ($R=0.53$) between biological activity and compounds pharmacophoric distances has been obtained. The proposed pharmacophoric designed model of effective congenic antidepressant drugs could benefit from using distance-based topography.

REVIEW REGARDING HUMAN METAPNEUMOVIRUS (hMPV), A SIGNIFICANT INFECTION OF THE RESPIRATORY TRACT

Sarfaraj Ahmad, Harsh Sharda, Kavita Joshi, and Vinita Pandey
Global Institute of Pharmaceutical Education & Research (GIPER)
Kashipur-244713, Uttarakhand, India

The virus known as human metapneumovirus (hMPV), which has been recognized in 2001, primarily affects infections of the upper and lower respiratory tract in youngsters, although it may also impact elderly people along with people with immune systems that are compromised. The primary causative agent for five to ten percent of children who are hospitalizations for severe infections of the respiratory tract is hMPV. Children who suffer from a hMPV infection can get severe bronchiolitis and pneumonia, and the symptoms are identical to those of a human respiratory syncytial virus, or HPV, infection. The first Infection with hMPV typically takes place in early childhood, although re-infections frequently happen at all ages. Because of the virus's sluggish growth in cell culture, molecular techniques (like reverse transcriptase PCR (RT-PCR)) are the favored diagnostic method for identifying hMPV. Several vaccine candidates have demonstrated effectiveness in preventing clinical disease, yet none are currently available for purchase. Our comprehension of hMPV has significantly evolved in recent years, and in this article, we will examine the existing data on the molecular biology and epidemiology of hMPV.

MOLECULAR DOCKING ANALYSES OF COMMON FOOD ADDITIVES HAVING GENOTOXICITY AND CHROMOSOMAL ABERRATION TARGET INTERACTIONS

Sisir Nandi, Sarfaraz Ahmed, Sombodhi Bhattacharya, and Anil Kumar Saxena

Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur-244713, India

Food additives have emerged as an essential element of the current food industry. They come from either natural or synthetic sources. Food additives are used specifically to keep food from spoiling, enhance its appearance, flavour, taste, texture, preservation and stabilization of the commercially available food for maintaining the freshness and nutritional value. But the uncontrolled uses of food additives are raising concern about their potential genotoxicity. Very frequently used food additives such as Disodium glycyrrhizate as sweetener, Sunset Yellow as coloring, Tartrazine as coloring, propyl gallate as antioxidant preservation and alloxan as wheat flour whitener may produce chromosomal aberrations and genomic instability. The molecular mechanisms behind these are yet to explore. An attempt has been made to compute the affinity of these food additives towards interacts with the genotoxicity and chromosomal aberration target proteins utilizing structure based docking simulations.

**PROVIDE AN OVERVIEW OF PBM, ITS HISTORICAL CONTEXT, AND ITS
SIGNIFICANCE IN CELLULAR HEALING**

Swati Tamta, and Shahjad

Global Institute of Pharmaceutical Education And Research College Of Pharmacy And
Research, Kashipur Uttarakhand 244713

A growing body of evidence supports the modulation of pain by light exposure. As such, phototherapy is being increasingly utilized for the management of a variety of pain conditions. The modes of delivery, and hence applications of phototherapy, vary by wavelength, intensity, and route of exposure. As such, differing mechanisms of action exist depending upon those parameters. Cutaneous application of red light (660nm) has been shown to reduce pain in neuropathies and complex regional pain syndrome-I, whereas visual application of the same wavelength of red light has been reported to exacerbate migraine headache in patients and lead to the development of functional pain in animal models. Interestingly visual exposure to green light can result in reduction in pain in variety of pain conditions such as migraine and fibromyalgia. Cutaneous application typically requires exposure on the order of minutes, whereas visual application requires exposure on the order of hours. Both routes of exposure elicit changes centrally in the brainstem and spinal cord, and peripherally in the dorsal root ganglia and nociceptors. The mechanisms of photo-biomodulation of pain presented in this review provide a foundation in furtherance of exploration of the utility of phototherapy as a tool in the management of pain.

HARNESSING COMPUTATIONAL POWER – A SYNERGISTIC CADD-AI APPROACH TO BREAST CANCER THERAPEUTICS

Vinita Pandey

Global Institute of Pharmaceutical Education & Research (GIPER)

Kashipur-244713, Uttarakhand, India

Breast cancer remains a significant global health issue. This challenge underscores the urgent need for novel therapeutic approaches. Computational drug discovery has advanced considerably, and Computer-Aided Drug Design (CADD) and Artificial Intelligence (AI) have emerged as powerful tools that accelerate drug development. This poster will examine the synergistic integration of CADD and AI in breast cancer therapeutics. CADD utilizes computational simulation methods, such as molecular dynamics to predict how prospective therapeutics interact with their biological targets. Additionally, AI tools are being incorporated to enhance prediction accuracy and improve insights into structure–activity relationships. AI-driven machine learning algorithms facilitate biomarker discovery, boost drug candidate optimization and aid target identification. These innovations decrease both time and expenses while enhancing accuracy. This approach leverages computational capabilities and holds significant promise for transforming breast cancer therapy and opens the door for targeted, more effective and personalized treatments.

ANTIMICROBIAL ACTIVITY OF AQUEOUS STEM EXTRACT OF CARICA PAPAYA AND RADISH LEAVES

Vivek kumar, Shahjad and Arun Kumar

**Global Institute of Pharmaceutical Education & Research, Kashipur, Uttarakhand,
India, 244713**

The stem of *Carica papaya* plant and radish leaves were collected and allowed to drying in dark place and ground in mortar pestle. The powdered material extracted successively using the maceration process with distilled water all the extract were subjected to systemic phytochemical screening for the presence of phytochemical constituent this indicate the presence of carbohydrate, protein, vitamin C, tannin, alkaloid, flavonoid. To verify the antimicrobial activity of all the extract were determine by cell wall diffusion method in the observation the stem of *Carica papaya* and radish leaves exhibit significant inhibitory activity against all the pathogen extract showed maximum activity. The sample further studied by FTIR it showed 13 functional groups in between the spectra 400 – 4000 nm.

ABSTRACTS OF E- POSTERS

EXPLORING NAV1.7 BLOCKERS IN ITCH MANAGEMENT: INSIGHTS FROM GX201 AND SULFAMETHOXAZOLE INTERACTIONS

Abhishek Kumar Mishra, and Sailendra Kumar Mahanta

The Assam Kaziranga University, Koraikhowa, NH-37, Jorhat 785006, Assam, India.

Pruritus, or itching, is a common symptom linked to dermatological and systemic conditions. NaV1.7, a voltage-gated sodium channel subtype, plays a pivotal role in transmitting itch signals through sensory neurons. Pharmacological research shows that inhibiting NaV1.7 can alleviate histamine-dependent itching, often triggered by allergic reactions or inflammation. GX201, a potent NaV1.7 blocker, has shown promise in managing neuropathic pain and reducing itch intensity by decreasing neuronal excitability. Sulfamethoxazole, an antibiotic used to inhibit bacterial growth, paradoxically induces itching through hypersensitivity reactions. These may involve either histamine release via immediate immune responses or cytokine-mediated inflammation in delayed-type reactions. Severe hypersensitivity can lead to conditions like Stevens-Johnson Syndrome (SJS) or Toxic Epidermal Necrolysis (TEN), further emphasizing the complexity of itching mechanisms. This study explores whether sulfamethoxazole binds to NaV1.7, similarly to GX201, and assesses its potential to alleviate itching through this pathway. Molecular docking analyses revealed that both compounds share the same NaV1.7 binding site but differ in binding energy, with GX201 exhibiting a stronger affinity (-9.29 kcal/mol) compared to sulfamethoxazole (-7.31 kcal/mol). Key interactions, such as hydrogen bonding, aromatic interactions, and hydrophobic effects, contribute to GX201's higher binding stability. Despite sharing a binding site, sulfamethoxazole's histamine-mediated itching underscores the limitations of targeting NaV1.7 alone. Effective itch management may require addressing additional pathways, including histamine receptor activation. These findings highlight the complexity of itch mechanisms and suggest that NaV1.7 inhibition, while promising, may not suffice as a standalone therapeutic strategy for comprehensive itch relief.

Keywords: NaV1.7 blockers, molecular docking, Itch, Neuropathic Pain, Docking energy

EXPLORING QSAR MODELING FOR A SERIES OF PYRAZOLE DERIVATIVES AS ACETYL CHOLINESTERASE INHIBITOR'S FOR THE MANAGEMENT OF ALZHEIMER'S DISEASE

Akshay Kumar, Jagadish Singh, and Partha Pratim Roy

Laboratory of Drug Discovery and Ecotoxicology, Department of pharmacy, Guru Ghasidas Vishwavidyalaya (A central University), Bilaspur, 495009, India

Alzheimer's disease is the most prevalent degenerative condition in the elderly, marked by symptoms such as dementia, memory impairment, and changes in behaviour, primarily caused by the degeneration of cholinergic neurons and other contributing factors. Heterocyclic compounds are crucial in the development of new drugs. Among these, pyrazole has emerged as one of the most researched and promising heterocyclic structures for treating Alzheimer's disease over the past decade with therapeutic effects against several key targets. The collected experimental data of 101 compounds targeting AChE was utilized for development of robust QSAR model. The developed models fulfil the good internal fitting ($R^2 = 0.692$; $R^2_{adj} = 0.675$), internal validation ($Q^2_{LOO} = 0.63$) external validation ($Q^2_{F1} = 0.795$, $Q^2_{F2} = 0.708$, CCC ext. = 0.871) MAE ext. = 0.246 and RMSE ext. = 0.322). Mechanistic interpretations highlighted the contribution of electropositive and bulky group at 3rd position of pyrazole scaffold. Chlorobenzene group at 2nd nitrogen of pyrazole is very essential for the activity. Electronegative group with fused aromatic ring enhanced the activity. Substitution with aromatic nitrogen fused heterocyclic compound at 3rd position of pyrazole drastically increases the activity. 2 H –Pyran attached with –NH₂ and CN group at 4th position of pyrazole responsible for increased activity. Overall, this research underscores the importance of the pyrazole scaffold in the treatment of Alzheimer's, showing potential for inhibitory action.

Keywords: QSAR, AChE, Alzheimer and Pyrazole

PHARMACOPHORE MODELING, 3-D QSAR, VIRTUAL SCREENING, DOCKING AND ADMET STUDIES OF QUINAZOLINE BASED EGFR INHIBITORS

Neelam Vashist, Aman Mudgal, and Arun Kumar

Department of pharmaceutical sciences, Gurugram university, Gurugram, Haryana, India-122018

Quinazoline is a special scaffold that can be structurally modified to generate new leads for drug discovery. Numerous tumor forms frequently exhibit increased EGFR expression, and this protein is being researched as a possible target for anticancer treatment. Pharmacophore modelling, virtual screening, molecular docking, 3-D QSAR and ADMET studies was performed to ascertain binding mode of quinazoline based EGFR inhibitors. Using dataset of 115 compounds a best model with four-point pharmacophore model (DRRR-1) was generated. This model was comprised of 1 hydrogen bond donor (D) and 3 aromatic rings (R) features which indicated importance of these interactions for the anticancer activity of quinazoline derivatives. A 3D-QSAR model with statistical significance was generated based on the pharmacophore concept. At the five component PLS factor, the model displayed a correlation coefficient of ($R^2 = 0.8328$), cross-validation coefficient ($Q^2 = 0.7120$), and F value (65.7). The generated 3D contour maps provided valuable insights into the structure-activity relationships of the compounds, aiding in the understanding of how specific structural modifications can impact their anticancer potential. To further explore the mode of action of these compounds, The PubChem database was screened against the DRRR_1 pharmacophore model. Following this screening, molecular docking analysis was performed, and the top five compounds were selected for further evaluation of their ADMET properties. Among these, compound CID 11488320 exhibited the highest docking score (-8.965 kcal/mol), suggesting a strong binding affinity to the target protein. Additionally, this compound demonstrated favourable hydrophobic interactions, further supporting its potential as an anticancer agent.

Keywords: Quinazoline, EGFR, Pharmacophore Modeling, 3-D QSAR, Virtual screening

TO EXPLORE PATHOGENESIS, CURRENT TARGETS AND MODE OF TREATMENT OF TRYPANOSOMIASIS

Astha Saha¹, Rukayya², Debapriya Ghosh¹, Ashaporna Biswas¹, Sujan Murmu¹, Amar Faruk Saheb¹, Tamanna Khatun¹, Barsha Roy¹, Asmita Samadder^{1,3} and Sisir Nandi^{2*}*

¹Cell and Developmental Biology Special, Department of Zoology, University of Kalyani, Kalyani, Nadia, 741235, India, ²Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur 244713, India, ³Cytogenetics and Molecular Biology Lab., Department of Zoology, University of Kalyani, Kalyani, Nadia, 741235, India

Trypanosomiasis is a parasitic disease caused by *Trypanosomabrucei* and *Trypanosomacruzi* responsible for producing Human African Trypanosomiasis (sleeping sickness), and American Trypanosomiasis (Chagas disease). Trypanosomiasis has been the prime concern for global health issues and has been designated as one of the seventeenth neglected tropical diseases (NTD) declared by the World Health Organization (WHO). Trypanosomiasis is most common among low-income countries and communities and claim immediate addressing to save lacks of lives of common human kind. However, there are no specific synthetic drugs known to cure the Trypanosomiasis. Existing chemotherapeutics are unable to kill the protozoa and therefore, the causative microorganisms become modified and transformed to more pathogenic forms. Therefore, this issue calls for prime exploration of the disease pathogenesis, and current targets for *Trypanosomabrucei* and *Trypanosomacruzi* for design and development of potent specific drugs targeting trypanosomal protozoa inhibition.

Key words: Trypanosomiasis, drug targets, pathobiology, essential proteins

NANOFORMULATION OF MORRONISIDE TO COMBAT DIABETIC NEPHROPATHY: A PROTEIN TARGETED EXPERIMENTAL APPROACH

¹*Banani Bhattacharjee*, ¹*Arnob Chakrovorty*, ¹*Asmita Samadder*, and ²*Sisir Nandi*

¹Cytogenetics and Molecular Biology Lab, Department of Zoology, University of Kalyani, Kalyani, Nadia, 741235, West Bengal, India

²Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research (GIPER) (Affiliated to Veer Madho Singh Bhandari Uttarakhand Technical University), Kashipur-244713, Uttarakhand, India.

Nanomaterials are used as therapeutic tools against myriads of diseases inducing diabetes. In the present study morroniside, a glycoside based phytochemical, was encapsulated in PLGA (poly-lactide-co-glycolide) to form nano-morroniside (NMOR) to check its potential against diabetic nephropathy. The physico-chemical properties of NMOR ascertained by FTIR provide an insight of the functional groups of morroniside present in the NMOR as spectral peaks and AFM study showed uniform spherical morphology with devoid of any cracks. Results of experimental study showed that NMOR worked better than un-encapsulated form of Morroniside by exhibiting an improved modulation of NF- κ B protein expression in renal tissue of Swiss albino mice *in vivo* to combat Diabetic nephropathy (DN). Data obtained from scanning electron microscope (SEM) showed protective efficacy of NMOR against alloxan (food additive) induced genotoxicity in HEK-293 cell *in vitro*. These data corroborated well with the results of blood glucose level, kidney function parameters assessed in *in vivo* model. Thus, the overall data suggests NMOR works as putative nano-therapeutics in preventing DN by targeting protein as regulatory factor.

Keywords: Nanoparticle, Diabetic nephropathy, Morroniside, Scanning electron microscopy, HEK-293

ENGINEERED ANTIBIOTICS: A STRATEGY TO COMBAT MULTI-DRUG-RESISTANT BACTERIA - ANTIBIOTICS MODIFICATION

*Bangmayee Dash¹, Susmita Chakrabarty¹, Nimay Chandra Giri², and Bhabani Shankar Nayak*³*

¹School of Paramedical and Allied Sciences, DRIEMS University Tangi, Cuttack-, Odisha, India.

²Department of Electronics and Communication EngineeringCenturion University of Technology and Management, Jatni 752050, Odisha, India.

³KIIT School of Pharmacy, KIMS, KIIT Deemed to be University, Campus-5, Patia, Bhubaneswar-751024, Odisha, India.

Drugs, which are known as antibiotics, treat bacterial infections in both humans and animals. A vast array of microorganisms, including fungi and bacteria, develop antibiotics. Mostly Antibiotics are getting ineffective as resistance developed by microorganism through changing and developing defense mechanism against Antibiotics. World Health Organization (WHO) predicts that antibiotic resistance could lead to 10 million deaths annually by 2050. Thus, it is going to a greater health issue in future. Contaminations brought on by drug-resistant bacteria have grown to be a significant problem for public healthcare systems in recent years. In actuality, the introduction of antibiotics has contributed to the rise of bacteria that are resistant to multiple drugs. In this study, we have tried to analyze detailed aspects of the antimicrobial resistance (AMR) mechanism conferred by both gram-negative and gram-positive bacteria by taking ESKAPE i.e., *E. coli*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, and *Pseudomonas aeruginosa*, *Enterobacter spp.* respectively. Herein, discussed novel redesigning methods for conventional antibiotics and provided a viewpoint on the subject. There is an acute need to discover and utilize unconventional methods for antibacterial drug development to block and tackle these global threats. It is essential to reduce the excessive use of antibiotics and reduce the possibility of unknown MDR bacteria. Furthermore, it is important to discover new classes of modified antibiotics to enhance the antibiotic's lifespan and deal with MDR bacteria.

Keywords: Antibiotic, Antimicrobial resistance, Multi-Drug-Resistant Bacteria, Biofilm & Drugs Modification.

EXPLORING THE ANTIBACTERIAL POTENTIAL OF PLANT-DERIVED BIOACTIVE COMPOUNDS IN FOOD PRESERVATION

Debasish Tripathy¹, Ishika Mandal², Deep Talukder², Bhabani Shankar Nayak^{3}, and Dhorodatta Senapati³*

Department of Pharmacology, Biju Patnaik University of Technology, Rourkela-769015, Odisha, India.

School of Biotechnology, KIIT Deemed to be University, Bhubaneswar-751024, Odisha, India.

KIIT School of Pharmacy, KIMS, KIIT Deemed to be University, Bhubaneswar-751024, Odisha, India.

Food preservation is a critical aspect of ensuring food safety and security, and the escalating demand for natural and sustainable antimicrobial agents has led to an increased focus on plant-derived bioactive compounds. A comprehensive analysis of recent studies is presented, encompassing the extraction methods, chemical diversity, and mechanisms of action of these bioactive compounds. The review highlights the rich repertoire of phytochemicals, including Phenolic, Alkaloids, Terpenoids, and essential oils, sourced from various plant species. These compounds exhibit notable antibacterial activities against a spectrum of food borne pathogens. Emphasis is placed on elucidating the mechanisms underlying the antimicrobial actions, such as disruption of cell membranes, interference with bacterial biofilm formation, and modulation of essential bacterial enzymes. Furthermore, the potential synergistic effects of combining multiple plant-derived compounds or integrating them with conventional preservatives are explored, aiming to enhance the overall antimicrobial efficacy and overcome potential limitations. The impact of extraction methods on the bioactivity of plant-derived compounds is discussed, with a focus on optimizing extraction processes for maximal preservation of bioactive properties. In addition, the review examines the practical applications of these plant-derived compounds in food preservation, considering factors such as dosage, stability, sensory attributes, and regulatory aspects. Current challenges and future directions in the utilization of plant-derived bioactive compounds for food preservation are critically discussed, providing insights into the potential development of novel and effective preservation strategies with minimal impact on food quality and safety. Overall, this review contributes to the growing body of knowledge on sustainable and natural alternatives in food preservation, fostering advancements in the field of antimicrobial research and technology.

Keywords: Antibacterial, Bioactive, Food Preservation, bacterial biofilm.

QBD BASED EXTRACTION OF PLUMBAGIN FROM PLUMBAGOINDICA ROOTS AND ITS ANTIOXIDANT ACTIVITY

Gayatri Khosla^{1}, Neeraj Kumar², Disha Dutta³, and Rama Tyagi¹*

¹Galgotias College of Pharmacy, Greater Noida, Uttar Pradesh, India, 201310

²Department of Pharmacognosy and Phytochemistry, School of Pharmaceutical Education & Science, New Delhi, 110062

³Devsthali Vidyapeeth College of Pharmacy, Rudrapur, Pin- 263148, Uttarakhand, India.

Plumbagin, a naphthaquinone found in *Plumbago Indica* roots, has various therapeutic characteristics. The research evaluates the effectiveness of several contemporary and traditional plumbagin extraction techniques. To optimize procedure variables for plumbagin extraction from *Plumbago Indica* roots, Box-Behnken Design (BBD) was used. Quality by Design (QbD), more especially BBD, was used to optimize extraction parameters (extraction time, solvent-to-drug ratio, and extraction temperature). Using HPTLC, the amount of plumbagin in various extracts was quantified. Moreover, the DPPH method was used to evaluate the antioxidant properties of several *Plumbago Indica* extracts. Methanol is an exceptionally efficient extractive solvent, and the ultrasound-assisted extraction approach yields the maximum amount of plumbagin. The ideal extraction temperature for plumbagin was determined to be 68.489°C, the solvent-to-drug ratio to be 31.249 mL/g, and the extraction duration to be 35.682 minutes using BBD. The yield of plumbagin under these circumstances was 1.981 mg/g, almost identical to the expected value of 1.893 mg/g. With a 79.39% percentage inhibition, the ethanolic extract has demonstrated notable antioxidant activity. Methanol was found to be the most effective extracting solvent, and the ultrasound-assisted extraction method was the most effective of all the thermal and non-thermal extraction techniques employed. The current work emphasizes the application of QbD, in the extraction field of therapeutically active phytoconstituents, which reduces the time and effort required for optimization.

Keywords: Response surface approach, extraction, optimization, plumbagin, and *plumbagoindica*.

IMPACT OF ANTIMICROBIAL RESISTANCE (AMR) AND STRATEGIC INTERVENTIONS: THE EVOLVING ROLE OF THE PHARMACEUTICAL SECTOR

*Mayank Kumar Khede^{*1,2}, Bhabani Shankar Nayak^{2,3}*

1 Biju Patnaik University of Technology, Rourkela - 769015, Odisha, India

2 Institute of Pharmacy and Technology, Salipur, Cuttack – 754202, Odisha, India.

3 KIIT School of Pharmacy, KIMS, KIIT Deemed to be University, Bhubaneswar-751024, Odisha, India.

Antimicrobial resistance (AMR) is a growing global health crisis that threatens the efficacy of existing antibiotics, leading to increased morbidity, mortality, and healthcare costs. The pharmaceutical sector plays a pivotal role in addressing this challenge through innovative drug development, antimicrobial stewardship, and policy advocacy. This article highlights the impact of AMR on healthcare systems, patient outcomes, and pharmaceutical sustainability, while highlighting strategic interventions for containment. Key approaches include the AWARe classification of antibiotics, implementation of national action plans (NAP-AMR), and infection prevention and control (IPC) programs. Advancements such as pharmacovigilance systems, rapid diagnostic technologies, and novel antimicrobial formulations, including nanotechnology-based drug delivery, are critical in optimizing antibiotic use. Additionally, the pharmaceutical industry must emphasize sustainable antibiotic production, ethical marketing, and collaborative research. Retail chemists and pharmacists serve as key players in antibiotic stewardship by ensuring responsible dispensing, patient education, and adherence monitoring. Regulatory bodies such as the Food and Drug Administration (FDA) play a crucial role in enforcing stringent regulations, monitoring antibiotic sales, and restricting over-the-counter misuse. By integrating policy-driven solutions, technological innovations, regulatory oversight, and industry-led commitments, the pharmaceutical sector can drive significant progress in AMR containment. Strengthening collaborations among healthcare professionals, policymakers, and pharmaceutical stakeholders is essential to safeguarding effective antimicrobial therapies for the future.

Keywords: Antimicrobial Resistance (AMR), Antibiotic Stewardship, Pharmaceutical Innovations, Regulatory Policies, Sustainable Antibiotic Use.

LIMONENE: A VERSATILE INGREDIENT IN THE COSMETIC INDUSTRY

Mohd.Tafseel, Disha Dutta, and Ramsha Aslam*

Devsthal Vidyapeeth College of Pharmacy Rudrapur, Uttarakhand

Limonene, a naturally occurring monoterpene hydrocarbon that is mostly derived from citrus fruits, has drawn a lot of interest in the cosmetics business. This substance has several advantages, such as a nice scent, antibacterial properties, and possible skin benefits. Because of its invigorating aroma, limonene is a common ingredient in body care products, colognes, and perfumes. Customers' whole sensory experience is improved by its zesty scent, which is frequently connected to freshness and cleanliness. In addition to its aroma qualities, limonene has antibacterial activity against a variety of microorganisms, which makes it a possible component of skincare products to help stop the growth of fungi and bacteria. Limonene has been researched for its possible advantages for skin health in addition to its scent and antibacterial qualities. According to some research, limonene may have antioxidant qualities that help shield the skin from harm brought on by free radicals. Its ability to increase skin suppleness and lessen wrinkle appearance has also been examined. To completely comprehend the mechanics underlying these possible advantages, more research is necessary. Because of its versatility, limonene is used in a variety of cosmetic items, such as body lotions, soaps, hair care products, colognes, and perfumes. It is anticipated that limonene's use in cosmetics would rise in tandem with consumer demand for sustainable and natural components. However, it is crucial to remember that limonene might irritate certain people, so its application needs to be carefully thought out, particularly in products meant for delicate skin.

Keywords: limonene, cosmetic industry, fragrance, antimicrobial, skin benefits.

EMULSOMES FOR TREATING DERMATOPHYTIC FUNGAL INFECTION— PREPARATION & EVALUATION METHODS THEREOF

Anish Menon¹, and Neha Mathur^{1}*

¹Amity Institute Pharmacy, Lucknow, Amity University Uttar Pradesh, Sector 125, Noida, 201313, India.

^{1*}Amity Institute Pharmacy, Lucknow, Amity University Uttar Pradesh, Sector 125, Noida, 201313 India.

Fungal infections, particularly dermatophytic infections, represent a significant global health challenge, affecting 20–25% of the population and contributing to a high mortality rate. Resistance mechanisms, including efflux protein overexpression, antifungal target mutations, biofilm formation (Dermatophytoma), and cross-resistance to allylamines and azoles, exacerbate treatment challenges.

Aim: -This study aimed to develop a lipid-based vesicular system, emulsomes, loaded with Atorvastatin and Eugenol, for topical application to address resistance and enhance antifungal efficacy.

Methodology:- Compatibility studies using FTIR confirmed the compatibility of Atorvastatin with lipids such as soya lecithin, cholesterol, and stearic acid, validating their suitability for emulsome formulation. Optimized Atorvastatin-Eugenol Emulsomes (ATS-Eu-EMLs) were prepared using the thin-film hydration method.

Results:-The prepared emulsomes demonstrated favorable characteristics, including an average size of 396.2 nm, a polydispersity index of 0.413, a zeta potential of –26.6 mV, and an entrapment efficiency exceeding 82%. Drug release studies showed sustained release of Atorvastatin from ATS-Eu-EMLs, with 39.24% release over 24 hours, following zero-order kinetics ($R^2 = 0.9984$), highlighting controlled release properties. *In vitro* antifungal studies against *Trichophyton rubrum* revealed superior efficacy of ATS-Eu-EMLs with a zone of inhibition of 13.9 mm, outperforming standard formulations.

Conclusion:-These findings demonstrate the potential of ATS-Eu-EMLs for effective management of dermatophytic fungal infections by enhancing drug retention, controlling release, and improving antifungal activity. The study successfully establishes a stable emulsome system for potential incorporation into suitable topical therapeutic applications.

Keywords: Fungal infections, Dermatophytic fungal infections, emulsomes, Atorvastatin, emulsomes.

UNVEILLING THE THERAPEUTIC POTENTIAL OF LULICONAZOLE

Pallavi Suyal, Disha Dutta, and Ramsha Aslam*

Devsthali Vidapeeth College of Pharmacy, Rudrapur, Uttarakhand

Luliconazole is a novel antifungal agent from the azole class, designed for topical application in the treatment of dermatophyte infections. It is primarily used in tinea pedis, tinea cruris, and tinea corporis. Luliconazole's therapeutic antifungal activity may be due to its significant in vitro activity and favourable pharmacokinetic characteristics in the skin. In 2005, Japan approved luliconazole 1% cream for the treatment of tinea infections. Luliconazole is an effective and safe topical treatment for dermatophyte infections providing rapid clinical resolution with minimal side effects. Luliconazole is classified as class II in the Biopharmaceutical Classification System, with minimal water solubility. Although it is accessible as a 1% w/v topical cream, its drawbacks include reduced skin permeability and shorter skin retention. Luliconazole is an antifungal agent from the imidazole class, notable for its distinct structure, which features the imidazole component integrated into the ketene dithioacetate framework. As the R-enantiomer, luliconazole exhibits greater antifungal efficacy compared to lanoconazole, a compound that exists as a racemic mixture. This review aims to encapsulate the in vitro findings, animal research, and clinical trial outcomes related to topical luliconazole usage. Preclinical investigations have shown remarkable effectiveness against dermatophytes. Additionally, both in vitro and in vivo research has indicated positive results against *Candida albicans*, *Malassezia* spp., and *Aspergillus fumigatus*. Though it is classified under the azole category, luliconazole possesses robust fungicidal properties against *Trichophyton* spp. The robust antifungal effectiveness of luliconazole may be due to a combination of its potent in vitro antifungal properties and advantageous pharmacokinetic characteristics within the skin. Clinical studies have shown that it is more effective than a placebo in treating dermatophytosis, and its antifungal potency is comparable to, or even exceeds, that of terbinafine.

Keywords: Luliconazole, Antifungal, Pharmacokinetic, Dermatophyte, Therapeutic.

**SYNTHESIS AND ANTIMICROBIAL EVALUATION OF NOVEL
DIOXOSPIRO[INDOLINE-3,2'-THIAZOLIDIN]-3'-YL)THIOUREA AND
-DIOXOSPIRO[INDOLINE-3,2'-THIAZOLIDIN]-3'-YL)UREA**

*Tandarani Ghosh,¹ Parhvini Awasthi², Ayshi Sahu¹, R.P Tiwari,¹ R.B Singh,¹ Krishna
Srivastava^{*1}, Nitin Srivastava^{2*}*

¹Faculty of Chemical Sciences, S R M University, Lucknow-Dewa Road, Barabanki. 225
003, India

²Department of Chemistry, Amity University Uttar Pradesh Lucknow Campus-226028,
India

The manuscript represents the preparation of 1-(1-(4-chlorophenyl)-1H-naphtho[1,2-e][1,3]oxazin-2(3H)-yl)-3-(2,4'-dioxospiro[indoline-3,2'-thiazolidin]-3'-yl)urea and 1-(1-(4-chlorophenyl)-1H-naphtho[1,2-e][1,3]oxazin-2(3H)-yl)-3-(2,4'-dioxospiro[indoline-3,2'-thiazolidin]-3'-yl)thiourea derivatives and their antimicrobial evaluation. Initially a series of Schiff bases was formed by the reaction of isatin with semicarbazide and thiosemicarbazide which was then subjected to undergo reaction with thioglycolic acid to form cyclized spiro derivatives. The cyclized derivatives were then reacted with substituted aryl aldehydes and β -naphthol under reflux conditions. Finally, the resulting cyclized derivatives of oxazine were formed by reaction of acetonitrile and formaldehyde. All newly synthesized derivatives conformation were characterized in detail by FT-IR and NMR spectroscopy including U-Visible and mass spectrometry. All the prepared derivatives exhibited good to excellent antimicrobial activities with MIC in appreciable range.

Keywords: Isatin, urea, β -naphthol, thiourea, acetonitrile, formaldehyde, thioglycolic acid, substituted aromatic-aldehyde.

BIOFILM FORMATION IN GASTRIC MUCOSA BY *HELICOBACTER PYLORI* INFECTION AND ITS ROLE IN DRUG RESISTANCE

*Pratyusa Biswas, and Laishram Pradeepkumar Singh**

Laboratory of Translational Biology and Molecular medicine, Department of Zoology,
University of Kalyani, Kalyani, Nadia- 741235

Helicobacter pylori is the most common, significant pathogenic agent which exhibits global prevalence of approximately 50%. It is associated with several gastrointestinal disorders including peptic ulcer and gastric cancer. Due to the highly increasing rate of infection the *H. pylori* eradication is the most necessary step to decrease the rate of gastric and duodenal ulcer and the gastric cancer prevalence. Despite of having different antibiotic-based medications, the treatment of *H. pylori* infection is hindered due to the emergence of antibiotic-resistance strain throughout the world. One of the most important mechanisms of drug resistance of *H. pylori* include formation of biofilm in gastric mucosa. During infection, some bacteria enter and occupy the gastric epithelium and encase themselves in an extracellular polymeric substances, known as biofilm. The biofilm structure that protects the bacterial colony from any external threat, is responsible for chronic infection of GI tract. Bacterial colony, covered with biofilm is 1000 times more resistant to any antibiotics than planktonic bacteria. Therefore, biofilm can be a novel therapeutic target to reduce the burden of drug-resistance infection of *H. pylori*. This review focuses on the molecular mechanism of biofilm formation of *H. pylori* in gastric mucosa including regulation by quorum sensing. Furthermore, it examines the clinical implications of biofilm-associated drug-resistance. Emerging therapeutic strategies targeting biofilm disruption are also discussed as potential solutions to overcome treatment failure. Understanding the intricate relationship between biofilm formation and drug-resistance offers valuable insights into developing more effective strategies to combat *H. pylori* associated diseases.

Keywords: *Helicobacter pylori*, biofilm, drug-resistance, infection, anti-biofilm agents.

FORMULATION AND EVALUATION OF BERBERINE CONTAINING NANO INVASOMAL VESICLES

Preeti^{1} Dinesh Puri²*

¹Siddhartha institute of pharmacy

²Graphic Era Hill University, Dehradun, Uttarakhand, India

Isoquinoline alkaloid berberine has a variety of medicinal uses but its applications have been hampered by factors such as low bioavailability, minimal absorption, and poor water solubility. Therefore, the goal of this work was to create optimal nanosized berberine invasomes with improved transdermal delivery to overcome the obstacles. The following formulation parameters were investigated by preparing berberine invasomes using a Box-Behnken experimental design: phospholipids %(x_1), terpenes %(x_2) and terpenes type (x_3) on entrapment efficiency (y_1) and vesicle size(y_2). On the bases of entrapment efficiency inva 21 and inva 27 were found best. The entrapment efficiency was 77 and 78 respectively. Inva 27 was further evaluated for particle size by dls. Particle diameter of inva 27 was 322.0 nm and polydispersity index were 0.2. The study's findings suggest that invasomes have a high potential for transdermal administration of berberine which can increase the topical utility of berberine in several skin diseases.

IN SILICO DESIGN AND EVALUATION OF TRPV1 INHIBITORS BASED ON CAPSAICIN FOR NEUROPATHIC PAIN

Priyakshi Chutia, and Sailendra Kumar Mahanta

The Assam Kaziranga University, Koraikhowa, NH-37, Jorhat 785006, Assam, India.

Neuropathic pain, a debilitating condition resulting from nerve injury, often involves the overactivation of the transient receptor potential vanilloid-1 (TRPV1) receptor, commonly known as the capsaicin receptor. TRPV1 is a non-selective cation channel activated by noxious stimuli such as heat, acidic pH, and capsaicin. It plays a central role in nociceptive signaling, inflammatory pain, and hyperalgesia. Targeting TRPV1 offers a promising therapeutic avenue for managing chronic pain conditions. This study focuses on the in silico design and evaluation of TRPV1 inhibitors derived from capsaicin, aiming to identify potent and selective modulators of this receptor. Computational approaches, including molecular docking, binding site and pocket analysis, and ADMET profiling, were utilized to design and assess the efficacy of novel TRPV1 inhibitors. Existing TRPV1-targeted therapies include both agonists and antagonists. While antagonists like AMG 517 and SB-705498 show efficacy in neuropathic pain management, challenges such as hyperthermia and off-target effects limit their clinical use. Conversely, agonists like capsaicin and resiniferatoxin (RTX) offer prolonged desensitization of nociceptive neurons, providing sustained analgesia. RTX, an ultrapotent capsaicin analog, demonstrates efficacy in preclinical and clinical studies for neuropathic pain, cancer pain, and inflammatory hyperalgesia. Despite promising advancements, translating TRPV1 modulators into clinical practice requires overcoming challenges such as irritancy, thermoregulatory side effects, and selectivity. This study highlights the potential of rational drug design in developing safer, more effective TRPV1 inhibitors for neuropathic pain, emphasizing the importance of computational approaches in accelerating drug discovery.

Keywords: TRPV1 receptor, Neuropathic pain, Capsaicin, Resiniferatoxin (RTX), Molecular docking, Rational drug design.

UNMASKING *LEISHMANIA DONOVANI* MAP KINASE12: COMPREHENSIVE STUDY IMPLIES IT'S PROBABLE ROLE AS A DRUG TARGET

*Priyanka H. Mazire**, Amit Roy

Department of Biotechnology, Savitribai Phule Pune University (Formerly University of Pune), Ganeshkhind Road, Pune- 411007, Maharashtra, INDIA

Visceral leishmaniasis (VL), a potentially fatal vector-borne disease, which is caused by the intracellular protozoan parasite *Leishmania donovani*, remains a major health problem due to restricted repertoire of drugs, deleterious side effects, high cost and drug resistance. So, there is an instantaneous need not only to search and design new efficacious affordable therapeutic agents with minimal side effects, but also to identify and validate newer drug targets for novel drug development. Mitogen-Activated Protein Kinases (MAPKs) are potential drug targets as they are regulators of diverse cellular processes. In this present study, we report *L. donovani* MAPK12 (LdMAPK12) as a probable virulence factor implying it as a plausible drug target. LdMAPK12 sequence is distinct from human MAPKs, while is highly conserved in different *Leishmania* species. It was observed that LdMAPK12 is expressed in both promastigotes and amastigotes. Higher expression of LdMAPK12 was seen in the virulent and metacyclic promastigotes in comparison with the avirulent and procyclic promastigotes. Furthermore, pro-inflammatory cytokines reduced, whereas anti-inflammatory cytokines increased LdMAPK12 expression in macrophages. Therefore, this study suggests a probable novel role of LdMAPK12 for parasite virulence and it can be exploited in near future as an important novel target for the development of new therapeutics for VL.

IN SILICO STUDIES OF 1,2,4-TRIAZOLE DERIVATIVES BY TARGETING DHFR AGAINST STAPHYLOCOCCUS AUREUS: PHARMACOPHORE GENERATION, ATOM-BASED 3D-QSAR, MOLECULAR DOCKING AND ADMET

Saket¹, Ankush¹, Arun Kumar¹, and Neelam Vashishth^{1}*

Department of pharmaceutical sciences, Gurugram university, Gurugram, Haryana, India-122018

Antibiotics, which disrupt essential processes for bacterial growth and proliferation, are crucial in combating bacterial infections. However, their misuse and overuse have resulted in increasing antimicrobial resistance, highlighting the urgent need for new antibiotics. Compounds with a 1,2,4-triazole ring exhibit diverse biological activities, with extensive research demonstrating their significant antimicrobial properties. *in silico* approaches are used on previously synthesized ninety-five 1,2,4-triazole derivatives against *staphylococcus aureus* for protein Dihydrofolate reductase. The protein Wild-type *staphylococcus aureus* DHFR in complex with NADPH and trimethoprim (PDB ID 2W9G), were used for the model development against the *S. aureus*. Alongside, the four features Ligand based pharmacophore hypothesis and Atom based 3D-QSAR model was generated with statistical parameters include correlation coefficient for the training set ($Q^2=0.7995$), regression coefficient for test set ($R^2=0.9808$) which proves the reliability of model. Contour visualization was done for the best docked and least docked compound. Furthermore, the best docked molecule was taken and through ChEMBL database ligand based virtual screening was performed. Later, ADME/T studies were carried out on top 5 compounds from the virtual screened database. Among the five compounds, the compounds ChEMBL 208844 and ChEMBL 275068 were found to be most potent antimicrobial agents against *S. aureus*. These compounds may be considered as lead for further development of antimicrobial agents.

Keywords: 1,2,4-triazole; antimicrobial activity; Atom based 3D-QSAR; Dihydrofolate Reductase; ADME/T.

EVALUATION OF ANTIFUNGAL POTENTIAL OF LANSOPERAZOLE: A DRUG REPURPOSING APPROACH

Sarita^{1*}, Neha Mathur¹, and Pooja Chawla²

^{1*}Amity Institute of Pharmacy, Amity University Uttar Pradesh, Lucknow- 226010, Uttar Pradesh, India; ²Baba Farid University of Health Sciences Faridkot (Punjab)

The pharmacological options for fungal infections are restricted to azoles, allylamines, echinocandins, and similar categories of medications. The fungal strain exhibits resistance to these treatment classes; hence, we employed a drug repurposing strategy by investigating current medications to validate potential therapeutic advantages through computational methods.

Aim & Objectives: To assess the potential of the new antifungal medicine, we employed antiepileptic medications in this investigation, utilizing *in silico* methods and the protein of interest for validation. **Method:** Docking was conducted using PRinS3 (Prescience in silico Solution Suite) version V 2.1.0. The X-ESS application conducted molecular dynamics simulations on human lanosterol 14- α demethylase (PDB ID: 3LD6) and fungal lanosterol 14- α demethylase (PDB ID: 5V5Z). Subsequent *in vitro* investigations were conducted utilizing the fungal strains *Trichophyton rubrum*, *Microsporum canis* and *Epidermophyton floccosum* alongside typical pharmacological agents Ketoconazole and Itraconazole for comparative analysis. **Result:** Docking and molecular dynamics simulations demonstrated substantial binding energy against 3LD6 -8.25 kcal/mol & 5V5Z – 8.46 kcal/mol were found & form stable ligand protein complexes for both proteins. The *in vitro* activity was carried out for Lansoperazole & MIC value was found to be 200 μ g/ml against both dermatophytes *Trichophyton rubrum*, *Epidermophyton floccosum* & 150 μ g/ml for *Microsporum canis* while standard drug Ketoconazole against *Trichophyton rubrum* show MIC value as 25 μ g/ml Ketoconazole against *Epidermophyton floccosum* show MIC value 25 μ g/ml. Ketoconazole and *Microsporum canis* 100 μ g/ml. **Summary & Conclusion:** *In silico* and *in vitro* research indicate that Lansoperazole presents as a promising antifungal agent and serves as an alternate treatment for prevalent fungal strains.

Keywords: Docking, Drug repurposing, Resistance, Anti-fungal drugs, MIC.

EVALUATION OF PREVENTIVE EFFICACY OF DIFFERENT PHYTOCOMPOUNDS TO COMBAT HYPERGLYCEMIA IN MICE MODEL: A COMPARATIVE ASSESSMENT

¹*Sayoni Dam*, ²*Sujan Murmu*, ²*Amar Faruk Saheb*, ²*Tamanna Khatun*, ²*Barsha Roy*, ²*Astha Saha*, ²*Debapriya Ghosh*, ²*Ashaporna Biswas*, ¹*Banani Bhattacharjee*, ¹*Arnob Chakrovorty*,
³*Sisir Nandi**, and ^{1,2}*Asmita Samadder**

¹Cytogenetics and Molecular Biology Laboratory, Department of Zoology, University of Kalyani, Kalyani, Nadia 741235, India

²Cell and Developmental Biology special, Department of Zoology, University of Kalyani, Kalyani, Nadia 741235, India

³Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur 244713, India.

Nature and natural components have been in use from time immemorial for healing several ailments of humankind. Presently, pertaining to the side effects incurred by the use of chemicals in synthetic drug materials, people are more inclined towards the usage of natural Phyto-compound as therapeutic agent against myriads of diseases. In the present study two important Phyto-compound, Chlorophyllin (CHL) and Curcumin (CUR) which are our culinary companion and are easily available and affordable, have been used to investigate their efficacy against food additive induced hyperglycaemia and its associated complications. The results revealed that both the Phyto-compounds were effective in inhibiting ROS generation in pancreas and liver and could restrict hyperglycaemia induced damage in the morphology of both the tissues. Additionally, the architecture of brain and testes were also restored by these Phyto-compounds even after initiation of hyperglycaemia in the experimental model. CHL and CUR also effectively inhibited the frequency of formation of comet tailed pancreatic cells when pre-treated prior to hyperglycemic induction. Although both the drugs showed similar results however, the results obtained from the comparative assessment for both the Phyto-compounds showed better results for CHL treatment than that of CUR treated group in terms of inhibition of blood glucose level, ROS generation and other parameters related to hyperglycaemia. Therefore, this study definitely suggests a possibility of using these two Phyto-compounds in the daily diet which would definitely help the diabetic patients to survive better with a longer life.

Keywords: Curcumin, Chlorophyllin, Hyperglycaemia, Phyto-compound, Reactive oxygen species generation.

SMALL MOLECULES FOR DRUG DEVELOPMENT OF ALZHEIMER'S DISEASE*Nitin Srivastava^{*}, Shivi Singh*

Department of Chemistry, Amity University Uttar Pradesh Lucknow Campus

Alzheimer's disease (AD) is the most common form of dementia and a challenging disease. It is characterized by cognitive decline, memory loss, and behavioural problems. The pathogenesis of AD is complex, and the molecular mechanisms and mechanisms involved in this devastating neurodegeneration are numerous. The development of small molecules targeting tauopathy and the search for antibodies are promising for the future of AD treatment. Here, we consider small-molecule therapeutics as a promising tool for the development of new drugs for the treatment of AD. Small molecules exhibit better shelf life, easier to handling and distribution, cheap, making them more suitable over the monoclonal antibodies. This review develops structural insight into the small molecules which have shown potential in drug development inhibiting the β -Amyloid ($A\beta$) and tau proteins responsible for protein misfolding along with overcoming oxidative stress, neuroinflammation, mitochondrial dysfunction and imbalances in cholinergic and glutamatergic tone. It may help the study of AD pharmacokinetics using small molecules, including new drug development, immunology, and clinical trial challenges.

Keywords: Alzheimer's disease, small molecules, β -Amyloid, Acetylcholinesterase, Tauopathy.

**DESIGNING, SYNTHESIS AND CHARACTERIZATION OF NOVEL
HETEROCYCLIC DERIVATIVES OF
-OXOTHIAZOLIDINE-3-CARBONYL)-6- SUBSTITUTED-SPIRO[INDOLINE-2,2'-
THIAZOLIDINE]-3,4'-DIONE AND -OXOTHIAZOLIDINE-3-CARBONOTHIOYL)-
6- SUBSTITUTED-SPIRO [INDOLINE-2,2'-THIAZOLIDINE]-3,4'-DIONE AND
THEIR BIOEVALUATION**

*Ayushi Sahu¹, Shreya Dwivedi², Anoop K. Awasthi³, Nitin Srivastava^{*2}, and Krishna
Srivastava^{*1}*

¹Faculty of Chemical Sciences, S R M University Lucknow-Dewa Road, Barabanki-225003,
India

²Department of Chemistry, Amity University Uttar Pradesh, Lucknow Campus-226028, India

³Department of Applied Science Rajkiya Engineering College, Mainpuri-205001, India.

A novel series of 3'-(2-(substituted-phenyl)-2-methyl-4-oxothiazolidine-3-carbonyl)-6-substituted-spiro[indoline-2,2'-thiazolidine]-3,4'-dione and 3'-(2-(substituted-phenyl)-2-methyl-4-oxothiazolidine-3-carbonothioyl)-6- substituted-spiro [indoline-2,2'-thiazolidine]-3,4'-dione derivatives were synthesized with good to excellent yield. The precursor imine has been formed by reaction of acetophenone with urea and thiourea. then reacting the resulting products with thioglycolic acid to yields thiazolidine-Carboxamide and thiazolidine-carbothioamide which again formed imine by the reaction of isatin to afford final spiro derivatives, further cyclization took place by the reaction of thioglycolic acid. The structures of the synthesized spiro derivatives were elucidated by their compatible spectral data given by U-Visible, Infra-Red-KBr, Proton Nuclear Magnetic Resonance and Mass. The reported compounds exhibited good antimicrobial activities with MIC ranging from 100.0 to 6.25 µg/mL.

Keywords: Urea, thiourea, acetophenone, isatin, pyridine, thioglycolic acid, zinc chloride.

COMBINATION OF SOLID DISPERSION AND POTENTIAL IONTOPHORESIS FOR IMPROVING TRANSCORNEAL *IN VITRO* PERMEATION 'OF ITRACONAZOLE

Swagatika Das¹, Biswaranjan Mohanty^{2}, Bibaswan Mishra³, and Bhabani Shankar Nayak^{4*}*

¹Himalayan Pharmacy Institute, Mjhitar, Rangpo, East Sikkim, India

²School of Pharmacy, DRIEMS University, Tangi, Cuttack, Odisha, India

³Institute of Pharmacy and Technology, Salipur, Cuttack, Odisha, India

⁴KIIT School of Pharmacy, KIMS, KIIT Deemed to be University, Bhubaneswar, Odisha, India

The delivery of medicament to eye faces difficulties due to the complex structure and presence of different static and dynamic barriers of eye. **Aim:** The present investigates improvement of the aqueous solubility of a poorly soluble itraconazole as solid dispersion with soluplus and to study the effect of different preservatives and application of iontophoresis on transcorneal permeation. **Methods:** Itraconazole solid dispersion was prepared and characterized by FTIR spectroscopy, differential scanning calorimetry and X-ray powder diffraction. **Results:** FTIR study revealed absence of any significant interactions between Itraconazole and soluplus. The drug was in an amorphous state or as a solid solution in the prepared solid dispersion supported by DSC thermograms and P-XRD study. The aqueous solubility of Itraconazole was found as $386.02 \pm 9.4 \mu\text{g/ml}$ from solid dispersion of drug to soluplus ratio 1:10. In-vitro transcorneal permeation showed maximum percentage permeation of itraconazole from the formulation containing BA (10.93 ± 0.14) followed by formulation containing MP+PP (7.94 ± 0.26) and BKC+EDTA (6.81 ± 0.19) after 2hrs. In iontophoretic study, increase in current intensity from 0.5 to 1.5 mA and iontophoresis time duration from 5 min to 15 min resulted in increased in drug permeation. Corneal hydration level was studied to assess the possible corneal damage due to electric treatment. The antifungal activity of the formulations against *Aspergillus flavus* determined by disk diffusion method suggested formulation containing BKC+EDTA showed the maximum zone of inhibition (14.33 ± 0.58 mm) compared to other formulations. **Conclusion:** Hence combinational effect of iontophoresis and BKC+EDTA as preservative has significant role enhancing the corneal permeation and antifungal activity that will potentially enhance the bioavailability of itraconazole to eye.

Key words: *Itraconazole; solid dispersion; transcorneal permeation; iontophoresis; antifungal activity.*

OBESITY - A REVIEW ARTICLE

**Swathi.V*¹, Dr. Sailendra kumar Mahanta², Dr.J.N.Suresh Kumar³, M.Harika⁴, Sk.Nagurbi⁴,
S.Suchitra⁴, V.Tharuni⁴,and P.Kethana Kumari⁴**

¹Associate Professor, Department of Pharmacology, Narasaraopeta Institute of
Pharmaceutical Sciences, Narasaraopet, A.P., India.

²Department of Pharmacology, School of Pharmacy, The Assam Kaziranga University

³Professor and Principal, Department of Pharmaceutics, Narasaraopeta Institute of
Pharmaceutical Sciences, Narasaraopet, A.P., India.

⁴Department of Pharmacy, Narasaraopeta Institute of Pharmaceutical Sciences,
Narasaraopet, A.P., India.

Obesity is an excessive accumulation of body fat, often induced by a BMI of 30 or higher. It increases the risk of health issues like heart disease and diabetes and is influenced by genetics, environment, and lifestyle choices. Obesity an intricate, multifactorial medical illness that presents substantial dangers to general health and is characterized by an excessive buildup of body fat. Increased risk of many chronic illnesses such as type-2 diabetes, cardiovascular diseases, certain malignancies and musculoskeletal disorders, has been connected to the syndrome. The etiology of obesity beside behavioral, environmental and hereditary factors. Modern lifestyles, marked by increased sedentary behavior and high-calorie, low-nutrient diets, exacerbate the risk of developing obesity. Addressing obesity requires a multifaceted approach including lifestyle modifications, dietary changes, physical activity and in some cases, pharmacological or surgical interventions. Prevention strategies exploit good diet and regular exercise. Effective management and prevention of obesity are crucial for reducing its burden on individuals and healthcare systems globally.

SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL SCREENING OF NOVEL HETEROCYCLIC DERIVATIVES OF OXAZINE AS 3-(SUBSTITUTED-PHENYL)-4-(3-(SUBSTITUTED-PHENYL)-3,4-DIHYDRO-2H-BENZO[E][1,3] OXAZIN-6-YL)-3,4-DIHYDRO-2H-NAPHTHO[2,3-E][1,3]OXAZINE

Krishna Srivastava,^{1} Vanshika Gupta², Ajay Kumar Tripathi¹, R.K Vishnoi², and Nitin Srivastava^{2*}*

¹Faculty of Chemical Sciences, S R M University Lucknow-Dewa Road, Barabanki. 225 003, India

²Department of chemistry, Amity University Lucknow Campous, Lucknow-226028 India

Innovative oxazin derivatives have been produced through one-pot, multicomponent condensation. The starting material oxazine-6-carbaldehyde was synthesized by the reaction of 1°amine and p-hydroxy benzaldehyde in toluene. **1a-c** further the condensation of carbaldehyde, substituted-1°amine and β-naphthol gives oxazin-6-yl)methyl)naphthalen-2-ol (**2a-l**) The obtained yields has been allowed to react with in acetonitrile to get target cyclized derivatives as 3-(4-bromophenyl)-4-(3-(4-chlorophenyl)-3,4-dihydro-2H-benzo[e][1,3]oxazin-6-yl)-3,4-dihydro-2H-naphtho[2,3-e][1,3]oxazine The structure of all the synthesized derivatives were elucidated by using FT-infrared(-ν max -cm⁻¹ -KBr), H NMR-CDCl₃ -300 MHz , mass spectral studies and antimicrobial activity in vitro studied by serial dilution method. The synthesized oxazin-derivatives exhibited significant antimicrobial properties against the tested microbes.

Keywords: Substituted 1°amine, β-naphthol, formaldehyde, oxazine, p-hydroxy benzaldehyde, toluene, acetonitrile.

