GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION & RESEARCH

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

Courses Offered

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

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- Special Atttention for 100% Placement
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- Dr. Anil Saxena, Chairman, ranked within top 2% scientist in the world in the field of Medicinal Chemistry as per Stanford University, USA

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Gold Medalist
M.Pharm (Pharm. Chemsitry), 2016-1018

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GTHTM-2024

INTERNATIONAL SYMPOSIUM ON GLOBAL TRENDS IN HEALTH, TECHNOLOGY & MANAGEMENT

March 15-17, 2024

Venue: Auditorium, VMSBUTU Dehradun, India

Organised By :

GLOBAL HEALTH TECHNO-MANAGEMENT FORUM (GHTMF)
GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION & RESEARCH (GIPER), KASHIPUR (US NAGAR), INDIA
VEER MADHO SINGH BHANDARI UTTARAKHAND TECHNICAL UNIVERSITY (VMSBUTU), DEHRADUN, INDIA

Website: conference.ghtmf.com, e-mail:gthtm2024@gmail.com, Ph. +917500458478

Our Sponsors

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Our Sponsors

From the desk of

Chairman (GTHTM-2024) and Organizing Secretary (GTHTM-2024)

Greetings, wish you all a good scene for an excellent end of 2024 with this International symposium (online and off-line mode) on Global Trends in Health, Technology and Management (GTHTM-2024) organized by Global Health Techno Management Forum, Global Institute of Pharmaceutical Education and Research, Kashipur and, Veer Madho Singh Bhandari Uttarakhand Technical University, Dehradun, India will be held at Dehradun from March 15-17, 2024.

The symposium is in continuation to our previous conferences such as the International Symposium on Drug Design and Development Research (DDDR-2021), International Symposium on Current Trends in Pharmaceutical and Medical Sciences (CTPMS-2020), International seminar on Global Trends in Health and Environment (2016), International Seminar on Pharmaceutical Education and Research (ISPER-2010), all of which were organized in GIPER, Kashipur and the 9th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2017) was organized at Goa. The GTHTM-2024 will bring together leading scientists, students, young pioneering minds both from academia industry, and corporate sector from different parts of the globe at a common platform to discuss the latest developments in the interdisciplinary fields of health, technology, and management covering a broad spectrum of topics like drug discovery and development including diseases like cancer, tropical and life style diseases, agroecology, artificial intelligence, machine learning, environmental protection, green agriculture, global warming, digitalization in health care, artificial intelligence, sustainable development goals and other areas pertaining to the theme of the symposium. The symposium will feature plenary lectures, oral talks and posters broadly covering the given fields.

We hope to offer you a memorable experience in exploring new ideas and opportunities. We thank all participants, speakers, honorable national and international advisory board members. Thanks to all staff members of the GIPER to make a grand success of this symposium.

Prof. Dr. Sisir Nandi
Organizing Secreatary
GTHTM-2024

Prof. Dr. Deepak Teotia
Chairman
GTHTM-2024

LT GEN GURMIT SINGH
PVSM, UYSM, AVSM, VSM (Retd)
GOVERNOR UTTARAKHAND

सत्यमेव जयते

RAJ BHAWAN
UTTARAKHAND
Phone : 0135-2757400
2757403

12 March, 2024

Message

It is interesting to note that the Veer Madho Singh Bhandari Uttarakhand Technical University is organizing an International Symposium on "Global Trends in Health, Technology and Management" (GTHTM-2024) in association with Global Techno Management Forum and Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur between March 15-17, 2024.

Global trends in health, technology, and management are rapidly evolving, reshaping industries and societies worldwide. In health, there's a shift towards personalized medicine, leveraging genomics and data analytics to tailor treatments. Telemedicine is also on the rise, improving access to healthcare, especially in remote areas. Technology trends like artificial intelligence (AI) and machine learning are revolutionizing management practices, enabling data-driven decision-making and automation of routine tasks. Virtual and augmented reality are transforming training and simulation in various industries, including healthcare and education. These trends highlight the need for continuous adaptation and innovation to stay competitive in the global landscape.

My best wishes to the organizers for the success of the international symposium, which will help accelerate sustainable growth in the field of health and its techno-management.

Gurmit

Lt Gen Gurmit Singh
PVSM, UYSM, AVSM, VSM(Retd)

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

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

Ref. No. 133/U.T.U/2024 Date. 06/03/2024

It is my great pleasure to note that **Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur** has formed an international forum by the name of Global Health Techno Management Forum (GHTMF) and is organizing an international symposium entitled **"International Symposium on Global Trends in Health, Technology and Management" (GTHTM-2024)** under the aegis of Veer Madho Singh Bhandari Uttarakhand Technical University from March 15-17, 2024. It makes a very good sense for excellent in the begining of 2024 because this both offline and online symposia will be a brain storming for the leading scientists, young researchers, academicians and students globally to create an open platform for discussing and resolving pertinent issues in the field of health, medicine, technology and management. I complement you all for the great efforts which may create enough well-trained human resources in the field so that these benefits are available to society all the time.

With warm wishes for the success of this symposia.

6/03/2024

Vice-Chancellor
Veer Madho Singh Bhandari Uttarakhand Technical University,
Dehradun, India

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. GIPER/2024/061 Date 13/03/2024

Prof. Dr. Anil Kumar Saxena, Ph.D., FRSC
Chairman, GIPER, Kashipur

Message

It is of immense pleasure that the Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur, has formed an international forum by the name of Global Health Techno Management Forum (GHTMF) and is organizing an international symposium entitled **"International Symposium on Global Trends in Health, Technology and Management" (GTHTM-2024)** under the aegis of Veer Madho Singh Bhandari Uttarakhand Technical Universityfrom March 15-17, 2024. The conference covers several topics under the broad research heads pharmaceuticals, medical and biomedical sciences, health and technology management, environmental protection, natural resources, green agriculture, cyber security, sustainable development goals, digitalization in health care and public health. The recent COVID-19 pandemic has shown the need for multi-sectoral coordination and collaboration when it comes to solving unpredicted challenges such as natural calamities or disease outbreaks. It will be useful toprovide a common platform for the innovative minds of a large number of eminent thinkers, scientists, educationists, business leaders, researchers and students to develop collaborative relationships among different specialities, industrial sectors and public-private organizations. One must think from a broader perspective and there is a need for collaboration at a global level. This International Symposium provides a platform to bring stakeholders from different fields of expertise to come together, exchange their ideas and work together for the betterment of society. I wish that due emphasis on these aspects shall be helpful to translate the real benefits of the current developments to the common man for improving health and the environment in which GIPER may play an important role. It is very graceful to combine the inauguration of this conference with the blessings of my mentor Dr. Nitya Anand who passed away at 99 years.

I welcome you all and look forward to your active participation in making this event a success. I take this opportunity to thank an elite gathering of scientists, educationists, business leaders and other professionals for taking pains to grace this occasion with their benign presence. I appreciate the sincere efforts of the members of the organizing committee and staff and students of the Global Institute of Pharmaceutical Education and Research, Kashipur and Veer Madho Singh Bhandari Uttarakhand Technical University for their active participation. I hope this event is a success.

Anil Kumar Saxena

Prof. Dr. Anil Kumar Saxena
Chairman

GTHTM-2024

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Prof. Alain Carpy (CNRS, Bordeaux, France)
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International Symposium on Global Trends in Health, Technology and Management (GTHTM-2024) (15-17March 2024)

Organized by

Global Health Techno-Management Forum (GHTMF)
Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur, and
Veer Madho Singh Bhandari Uttarakhand Technical University, Dehradun

Program Schedule

15 March 2024 (Day 1)

REGISTRATION	
Time	**Program**
14:00-16:00	Registration
INAUGURAL SESSION	
16:30	Arrival of Chief Guest (Hon'ble Governor, Uttarakhand)
16:30-16:35	Guard of Honour by NCC Cadets
16:35-16:40	Garlanding of statue of Veer Madho Singh Bhandari and Wall of Heroes
16:40	Arrival in Auditorium
16:40-16:41	National Anthem
16:41-16:42	Lamp Lighting & Saraswati Vandana
16:42-16:44	University Kulgeet
16:44-16:45	Presentation of bouquet and release of e-souvenir
16:45-16:50	Welcome by Vice Chancellor, VMSB Uttarakhand Technical University, Dehradun
16:50-16:55	Dr. Anil Kumar Saxena, Chairman, GIPER: Tribute to Dr. Nityanand and Dr. V.P. Kamboj
16:55-17:00	Brief speech by Dr. Soniya Nityanand, Vice Chancellor, King George Medical University, Lucknow
17:00-17:05	Brief speech by Dr. Omer Saka, Health Economist and Business Development expert, Switzerland
17:05-17:25	Address by the Chief Guest Hon'ble Governor, Uttarakhand

17:25-17:27	Presentation of Memento to Dignitaries
17:27-17:29	Vote of Thanks by The Registrar of VMSBUTU, Dehradun
17:29-17:30	National Anthem
17:30-17:50	High Tea
Scientific Session –I Chairpersons: Prof. Dr. Onkar Singh and Prof. Dr. Anil Kumar Saxena	
17:55-18:25	Keynote lecture: Dr Soniya Nityanand, Hon'ble Vice Chancellor, KGMU, Lucknow
18:30-19:00	Prof. Dr. Gunda Georg, USA: The male pill: Are we there yet?
19:10-20:30	Cultural programs

16 March 2024 (Day 2)

Scientific Session –II Chairpersons: Prof.Dr.AthinaGeronikakiandProf.Dr.Vineet Kumar		
Time	**Speaker**	**Title**
09:00- 09:20	Prof. Dr. Om Prakash, USA	Conquering the neutrophil-A tale of novel neutrophil serine protease inhibitors
09:20-09:40	Prof. Dr.Diwan Singh Rawat, India	Navigating the expected and unexpected twists and turns of lead optimization: The discovery of clinical candidate for the treatment of Parkinson's disease
09:40-10:00	Prof. Dr.Dmitry Druzhilovskiy, Russia	WAY2DRUG: Efficient prediction of biological activities from global to local scales
10:00- 10:20	Prof. Shubhra Ghosh Dastidar, India	Allosteric changes in proteins: Earning extra miles of understanding from MD simulations
10:20- 10:40	**Coffee/Tea Break**	
Scientific Session –III Chairpersons: Prof. Dr. Diwan Singh Rawat and Dr. Aaruni Saxena		
10:40- 11:00	Dr. Alok K. Saxena, India	Technologylife cycle – concept to commissioning
11:00- 11:20	Mr. Naveen PralhadDeshpande	Leveraging digital technology for public health emergency preparedness: A multi-level perspective
11:20– 11:40	Dr. Rahul Singhal, India	Heart problems in community
11:40– 12:00	Dr. Omer Saka, Switzerland	Digitalization in healthcare
12:00– 12:10	Dr. Amit Roy	Ritonavir enhances the efficacy of amprenavir in combination in clinically isolated *Leishmania* parasites
12:10– 14:00	**Poster session I and lunch** Committee for poster session assessment: Dr. Anshuman Dixit (Chairman), Dr. Gyan Prakash Modi, Dr. Shubhra Ghosh Dastidar, Dr. Amit Roy	
Scientific Session –IV Chairpersons: Prof. Dr. Arun Sinha and Prof. Dr. Indira Ghosh		
14:00 –14:20	Prof. Athina Geronikaki, Greece	Pyrazolo[4,3-c]pyridinesulfonamides as carbonicanhydrase inhibitors:synthesis, biological and *in silico*studies
14:20 –14:40	Dr. Sanjay Batra,India	Development of biasedKORagonist for managingchronicpain

14:40 –15:00	Dr. Anshuman Dixit, India	Identification of targeted therapeutics against oral squamous cell carcinoma
15:00 –15:20	Dr. Aaruni Saxena, UK	ONCORx: A digital App for cancer treatment planning
15:20-15:40	Mr. Atul Tripathi, India	Quantum computing and machine learning for drug discovery
15:40 –16:00	**Tea/coffee break**	
Scientific Session –V(online session) Chairpersons: Dr. Sanjay BatraandDr. Rakesh Shukla		
16:00– 16:20	Prof. B. Jayaram, India	The many facets of AI/ML along genome to drug pathway
16:20- 16:40	Dr. Marjan Vracko, Slovenia	'Big and small data' in computational modelling of toxicological endpoints
16:40– 17:25	Dr. Subhash C. Basak,USA and Dr. R. Natarajan, India	Numerical characterization of enantiomers and diastereomers for Quantitative Chiral Structure-activity Relationship (QCSAR) Modeling
17:25– 17:35	Dr. Indrani Bera, India	Proteolysis pattern of plant seed proteins; insight from the endogenous peptidome of germinated and ungerminated chickpeas using LC-MS/MS.
17:35– 17:45	Dr. Madhumita Dandopath Patra, India	Comparative analysis of ligand binding and role of metal ion in lectins using docking studies
17:45– 17:55	Ms. Asha Gummadi, India	Applications of artificial intelligence in the pharmacy sector
Scientific Session –VI (Oral presentation session) Chairpersons: Prof. Dr. Deepak Teotiaand Prof. Dr.Yusra Ahmad		
17:55– 18:05	Ms. Rishita Dey, India	Docking-based experimental approach examining the effectiveness of nano-formulations as diabetes therapeutics
18:05– 18:15	Ms. Sudatta Dey, India	Nano-phytocompound combats food-additive induced genotoxicity and mitochondrial dysfunction in the diabetic model: an *in silico* predicted experimental study
18:15–18:25	Ms. Sweta Bharadwaj, India	Xenobiotic-induced obesity associated male reproductive tract dysfunction in *Drosophila*
18:25– 18:35	Mr. Mayank Kumar Khede, India	Innovative approaches to climate-resilient healthcare: Harnessing the power of pharmacy
18:35- 18:45	Mr. Jeevan Patra, India	Structural binding modes and optimizations of dual falcipain inhibitors using computational approaches
18:45– 18:55	Mrs. Shivani Lodha, India	To determine the prevalence of psychoticillness in targetedpopulation
Online poster session Chairperson:Dr. AsmitaSamadder		
18:55 -19:00	Mrs. Aparna Joshi	Optimizing solubility through co-crystal technology: A rigorous investigation into tablets loaded with azelnidipine co-crystals
19:00 –19:05	Ms. Sarita	Comperative studies of some common FDA approved drugs against human and fungal protein
19:05 –19:10	Ms. Priyanka Tomar	Exploring the potential of herbal nano sponges in combating the skin infections
19:10 –19:15	Dr. Pradeep Pilania	Modeling of the cyclic guanidines as 5-HT_{5A} receptor ligands using chemometric tools

17 March 2024 (Day 3)

Scientific Session –VII Chairpersons: Dr. Alok SaxenaandProf. Dr. Dmitry Druzhilovskiy		
9:00 – 9:20	Prof. Dr.Indira Ghosh, India	Strategy to combat persistent Tuberculosis: Entrapment of the flow of substrate in the non-essential pathway
9:20 – 9:40	Prof. Dr. Prasad V. Bharatam, India	The importance of 3D thinking in anti-bacterial agent discovery
9:40 - 10:00	Prof. Dr. Anil Kumar Saxena, India	Quantitative Structure Interaction Activity Relationship (QSIAR): a novel approach to drug design: a case study of ani-tubercular agent
10:00 - 10:20	Prof. Dr.Arun K. Sinha, India	Green- and Click-Chemistry:An opportunity for simplification and innovation towards natural and nature-inspired synthetic small molecules of biological and commercial importance
10:20 - 10:40	Dr. AsmitaSamadder, India	Strategic formulation and evaluation of nano-insulin in combating arsenic-induced hyperglycemia in mice model.
10:40- 10:55	Dr. Gyan Prakash Modi, India	Development of natural template-based novel diagnostic andtheranostic agents and their formulation development for Alzheimer's disease
10:55-11:10	Dr. Avik Kumar Bagdi, India	Visible-Light-Mediated synthesis of functionalized heterocycles
11:10 -11:25	Dr Sisir Nandi, India	Structure-based exploration of common food additivesto combatchromosomal aberration
11:25 - 11:40	Dr Kuldeep Roy, India	Elucidation of the binding modes of known small-molecule inhibitors at mycobacterial ATPase synthase subunits *C*and *E*
11:40– 11:50	Dr. Smriti Arora, India	A designer diet for astronauts using the microbiomebased approach
11:50 -12:00	**Tea/Coffee break**	
12:00 -12:45	**Panel discussion (**Moderator: Dr. Aaruni Saxena)	How to build a resilient health system from drug development to healthcare delivery in a resource-scarce setting? **Panelists:**Dr. Omer Saka,Dr. AnilKumar Saxena, Dr. Suman Singhal
12:45- 13:15	**Valedictory session, award ceremony and vote of thanks**	
13:15– 14:00	**Lunch and dispersal**	

BIO SKETCHES

OF

RESOURCE PERSONS

Prof. Dr. Onkar Singh, Hon'ble Vice Chancellor,
VMSBUTU, Dehradun

Dr. Onkar Singh, honorable Vice Chancellor of Veer Madho Singh Bhandari Uttarakhand Technical University, was a Professor of Mechanical Engineering at Harcourt Butler Technical University (Formerly HBTI), Kanpur since 2007. He has been the founder Vice-Chancellor of Madan Mohan Malaviya University of Technology, Gorakhpur from 17th December 2013 to 28th April 2017. Dr. Singh has also been Vice-Chancellor of Uttar Pradesh Technical University, Lucknow from 30th April 2015 - 4th August 2015 and also held responsibility of Vice Chancellor of Veer Chandra Singh Garhwali Uttarakhand University of Horticulture and Forestry, Bharsar, Pauri Garhwal during 12th October 2022 to 16th December 2022. Dr. Singh has authored 12 books, edited 02 books, 6 conference proceedings, authored 13 book chapters He has published 233 papers in International/ National journal and 144 popular articles. Dr. Singh has guided 15 Ph.D. students, 29 PG dissertations, and completed 08 research projects. He possesses 03 patents, 01 copyright, and two National Records – LIMCA Book of Records, March 2014, and LIMCA Book of Records, February 2015. He is the governing body members of many eminent institutes and universities. He is Fellow of The Institution of Engineers(India), Fellow of Indian Society of Mechanical Engineers, Fellow of International Society for Energy, Environment and Sustainability, Honorary Fellow & Life Member of Indian Society of Technical Education, Life Member of Oil Technologists Association of India, Member of Indian Society of Heating and Refrigeration Engineers, Life Member of Indian Science Congress Association, Fellow of International Society for Energy, Environment and Sustainability and Member of American Society of Mechanical Engineers, USA. He is the recipient of the National Scholarship, AICTE Young Teacher Career Award in the year 2000, 100 Most Influential Vice Chancellors Award –2016, and Asia's Education Excellence Award – Exemplary Leader award – 2016.

Dr. Anil Kumar Saxena, Ph.D., FRSC

Dr. Anil Kumar Saxena, Chairman, Global Institute of Pharmaceutical Education and Research, Kashipur, Ex-Chief Scientist Central Drug Research Institute, Lucknow, India is actively involved in Medicinal Chemistry & Computer Aided Drug Design (CADD). He has more than 50 years of research experience, 230 research papers, 31 reviews/articles in books/monographs and 72 patents to his credit. He has delivered >190 invited lectures, chaired >55 session and has made >60 visits abroad. He has supervised >200 post graduates and 45 PhD students. Dr. Saxena has initiated QSAR and the concepts of CADD in early 70's and established it in CDRI and made major contributions for its development 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, an Honorary Medal for outstanding contributions to Medicinal Chemistry and International Scientific collaboration Moscow, Russia, 2004 and Prof. P.K. Bose Memorial Award (Indian Chemical Society, 2009), Edupreneur of the year (2019) and Life time achievement (2021) by Center for Education Growth and Research (CEGR). He is Fellow of Royal Society of Chemistry, UK, and is also series editor for book series "Topics in Medicinal Chemistry" published by Springer Verlag. 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. He has been member of several committees including Expert Committee, Ministry of Chemicals & Fertilizers, Department of Pharmaceuticals, IND Committee, CDSCO, Govt. of India, New Delhi, and American Chemical Society. It is noteworthy that Dr. Saxena has been enlisted for the 3rd consecutive year in the list of the top 2% scientist in the world Stanford University, USA.

Dr. Med. 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 Organisation 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.

Prof. Dr. Arun K Sinha, FNASc, FRSC

Dr. Arun K Sinha is former Pro Vice-Chancellor, Ranchi University, Ranchi, Jharkhand He was a Chief Scientist and Professor (ACSIR) in Medicinal and Process Chemistry, C.SI.R-Central Drug Research Institute (CDRI), Lucknow. He received his M. Sc. in 1984 from Banaras Hindu University, Varanasi and Ph.D. in 1990 from Indian Institute of Technology, Delhi in Organic Chemistry After exposure in industries for three years in India, he moved for his post doctoral research at Illinois Institute of Technology (IIT), Chicago and University of Illinois at Urbana Champaign (UIUC), Illinois, U.S.A during 1994-1997. Then, he returned back to India in 1997 and joined at CSIR-Institute of Himalayan Bioresource Technology, Palampur, H.P, India. During 2007-08, he was a visiting scientist at Umea University, Sweden. In 2013, he moved as a Chief Scientist to CSIR-Central Drug Research Institute, Lucknow (UP), India. His research interests focus on medicinal chemistry, natural products, biotransformation and green chemistry towards the development of step-economical synthesis of small molecules of commercial and biological importance. He has also received several awards and fellowships such as Fellow of National Academy of Sciences (FNASc), Allahabad in 2014, CRSI- Bronze Medal, Bangalore in 2012 and Dr. P. D. Sethi Award (for the best Indian research papers in Pharmaceutical Analysis, consecutive for four years) from 2009 to 2012. Dr. Sinha also has 118 publications and 17 patents to his name.

Dr. Amit Roy

Dr. Amit Roy is now UGC-Assistant Professorat Department of Biotechnology, Savitribai Phule Pune University, India. Before that he was Assistant Professor (2013 to 2017) in National Institute of Pharmaceutical Education and Research (NIPER), Hajipur, India. He obtained his Ph.Ddegree in 2009from Jadavpur University, Kolkata, India working in CSIR-Indian Institute of Chemical Biology, Kolkata.He was awarded Postdoctoral Fellowship from "Danish Cancer Society, Denmark"on February 2010 and Carlsberg Foundation, Denmark on January 2011. He has completed his postdoc from AarhusUniversity, Denmark in 2012. He is a recipient of INSA Young Scientist Award (2011) and Professor LSS Kumar Memorial Award (2011) by Indian National Science Academy (INSA), Govt. of India. He is the "Elected Member of Sectional Committee of the Section of Medical Sciences (including Physiology)" for 2023-2024 (109^{th}session of Indian Science Congress). His areas of specialization are Molecular Parasitology, Molecular Biology, Enzymology,Drug Developmentand Therapeutics. He has published 34 research papers in peer-reviewed international journals and 6 book chapters. He is the life members of different professional societies and editorial board members of different international journals.

Dr. Anshuman Dixit

Dr. Anshuman Dixit, a distinguished Scientist-D at the Department of Biotechnology, Institute of Life Sciences, Nalco Square, India, boasts a stellar academic background. He completed his Ph.D. in 2007 at the Central Drug Research Institute (CDRI), Lucknow, preceded by an M. Pharm in Pharmaceutical Chemistry and a B. Pharm in Pharmacy from Dr. H. S. Gour University, Sagar, M.P., India. Throughout his academic journey, Dr. Dixit has garnered prestigious fellowships including the Graduate Aptitude Test in Engineering-1997 (GATE-97) and the CSIR-Senior Research Fellowship (CSIR-SRF) in 2003. He holds life membership with the Indian Pharmaceutical Association and is affiliated with the American Chemical Society. With a solid foundation in research, Dr. Dixit has accrued over nine years of experience in the field. He spent five years conducting doctoral research at CDRI, Lucknow, and almost four years as a postdoctoral researcher at the University of Kansas, Lawrence, KS, USA. Dr. Dixit's research interests encompass a wide spectrum, including drug design and discovery, bioinformatics, and structural studies. Notable projects include investigations into C. albicans DNA Polymerases, structure-function analysis of CuZn-SOD in Ipomoea carnea, and modeling studies on A3AR receptors and TLRs. His work extends to virtual screening of chemical libraries to identify potential FtsZ inhibitors.His contributions to the scientific community reflect his dedication to advancing biotechnology. Dr. Dixit's expertise, honed through years of rigorous research, positions him as a notable figure in the field, poised to continue making significant strides in understanding and innovating within biotechnology.

Dr. Asmita Samadder 

Dr. Asmita Samadder, M.Sc., Ph.Dis working as an Assistant Professor, Department of Zoology, University of Kalyani, India. Citation: 2193, h index: 30, i-10 index: 46. 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 90 original research publications in International peer-reviewed journals of repute. Dr. Samadder served as an Assistant Professor and Head in the Department of Zoology, Dumdum Motijheel College, Kolkata, India from 2015-2018.Dr. Samadder works in the area of Nanotechnology and nano-medicine more than 16 years. Her research interest includes nano-formulation of several drugs to combat Diabetes and its associated complications like Alzheimers disease, diabetic kidney diseases, etc, along with other toxicological pathophysiology exploring well defined cytogenetics and molecular biology outreach. Dr. Samadder receivedmajor research grant from SERB (DST) and UGCGovt. of India. She is the winner of "Young Scientist Award" for her outstanding research paper presented in SYDNEY, AUSTRALIA in October, 2012 and Je Ma award at STOCKHOLM, SWEDEN in 2013. She was invited as resource person at the "International Integrative Medicine Expo" in JANGHEUNG, SOUTH KOREAin 2016. She is the Editorial Board member of several internal journals like, Journal of Cellular Biological and Molecular, Sciences (Ommega-Publishers), International Journal of Experimental Research and Review (International academic publishing house), Nano and Medical Material (Academic Publishing Pte Ltd), EC Pharmacology and Toxicology (ECronicon Journal Publishing house).

Dr. Alok Kumar Saxena 

Alok Saxena superannuated as Managing Director, Sulzer GTC India Pvt. Ltd six months ago. Presently proprietor -AA Consultants. He is a Chemical Engineer with Doctorate from IIT, Delhi and Post-Doctorate from University of Oldenburg, Germany. He has > 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 >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.

Prof. Dr. Athina Geronikaki

Athina Geronikaki graduated from Tashkent State University in 1971 and gained the specialty of organic chemist. In 1977 she defended her PhD thesis and received the Ph.D grade in Chemistry (Ph.D, 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. Her scientific interest is: Chemistry of natural products isolation, determination of structure; Chemistry of biologically active compounds and evaluation of their activity, using different computational methods. She organized five International conferences: Computational Methods in Toxicology and Pharmacology, Integrating Internet Resources (CMTPI) (2003) Thessaloniki; 4^{th} Eurasian Meeting on heterocyclic Chemistry , 2006 , Thessaloniki, 8^{th} CMTPI -2015 and 23^{d} Hellenic Symposium in Medicinal Chemistry, 2017, CMTPI-2019. Published more than 200 papers and 5 chapters in a book. Wrote 4 books for student. Has 23 Erasmus agreements and is University coordinator of Paul Ehrlich PhD Network in Medicinal Chemistry. She had several grants, among which are INTAS, Pythagoras and others.Several times she was awarded from International Scientific Foundation. She was invited speaker in 46 International conferences and in most of them member of Advisory and Scientific Board. She is member of Editorial Board in several journals (Molecules, Jordanian J .of Chemisstry, International Journal of Pharmaceutical Sciences Research, Diabetes& obesity International Journal, Journal of Drug Design and Research, APG-Austin Journal of Analytical & Pharmaceutical Chemistry), International Editor of Revista de Ciências Farmacêuticas Básica e Aplicada/ Journal of Basic and Applied Pharmaceutical Sciences, Advisory Board member of Chemistry & Biology Interface.Academic Editor in Molecules Executive editor in Current Topics in Medicinal Chemistry.

Mr. Atul Tripathi

Ex Big Data & AI consultant in National Security Council Secretariat (Prime Minister's Office, New Delhi, India)

He has 20+ years of experience in Artificial Intelligence, Big Data, Generative AI, UNSDG, ESG, Disaster Risk, Cyber security, Data Policy & AI Ethics. He has worked across Prime Minister's Office, Industry, R&D (IIT Kanpur, ISI Kolkata). Atul has been part of delegation where he has represented the country at various international forums and international negotiations. He works very closely with Government of India in advisory capacity to Government of India. His current research area is in Quantum Machine Learning and Generative AI. He has been teaching AI,Data Policy, AI Ethics, Insurance, Anti Money Laundering, Risk Managementand more at various universities, institutions and industries such as asIIITSricity, IIM Lucknow, IIM Indore, IIT Roorkee, BIMTECH, Goa Institute of Management, Indian Institute of Public Administration, ATI Nainital and more. He is an author of couple of books on AI. The book has been translated in Chinese and Korean.

Dr. Avik Kumar Bagdi

Dr. Avik Kumar Bagdi obtained his Ph.D. from the Department of Chemistry, Visva-Bharati, India in 2014 under the guidance of Dr. Alakananda Hajra. He received 2nd Prize of "2014 Eli Lilly & Company Asia Outstanding Thesis Award". In 2015, he was appointed as an Assistant Professor at the Triveni Devi Bhalotia College, Raniganj. In 2016, he went to OIST, Japan to carry out his Post-Doctoral Research with Prof. Fujie Tanaka. Since 2018, Dr. Bagdi is working as an Assistant Professor in the Department of Chemistry, University of Kalyani, India. His current research interest includes the employment of visible-light photocatalysis in the synthesis and functionalization of bio-active heterocycles.

Prof. Dr. B. Jayaram

Prof. B. Jayaram received his Ph.D. in 1986 from the City University of New York (CUNY, NY, USA) under the mentorship of Prof. David L. Beveridge. He then worked as a Post Doctoral Fellow (1987-88) with Prof. Barry Honig at Columbia University, NY, USA and as a Senior Research Associate (1989-1990) with Prof. Beveridge at Wesleyan University, CT, USA. In 1990, Prof. Jayaram joined IIT Delhi and worked as a (i) Faculty at IIT Delhi from 1990-2019, (ii) Emeritus Professor at IIT, Delhi from 2019-2023. He was (iii) Head of Chemistry Department, IIT Delhi (2006-2009), (iv) Founder Coordinator of Kusuma School of Biological Sciences, IIT Delhi (2008-2014), (v) Founder Coordinator of Supercomputing Facility for Bioinformatics & Computational Biology (SCFBio), IIT Delhi (2002-2019). Prof. Jayaram served as a member of the (vi) Physical Chemistry Programme Advisory Committee (PAC) of the Department of Science & Technology (DST), Govt. of India (2004-2007), (vii) Organic Chemistry PAC of DST (2007-2011), (viii) Bioinformatics Task Force of the Department of Biotechnology, Govt. of India (1998-2009 & 2013-2018), (ix) Bioinformatics Working Group of the Department of Information Technology, Govt. of India (2006-2013), (x) IUPAB National Committee (2008-2011), (xi) DST-FIST Committee for Chemical Sciences (2009-2010), (xii) Bioinformatics task force of ICMR (2012-2013), (xiii) DST PAC on Biochemistry, Biophysics & Molecular Biology (2013-2015). (xiv) He wasChairman of DBT's committee on promotion and popularization of Biotechnology (2009-2013) and (xv) Vice President of Indian Biophysical Society (2007-2009). He is currently a (xvi) Co-Chair, Data Management Committee, DBT (2024-2027). He has been Editorial Board of emiment journals like Journal Proteins & Proteomics, Journal of Bioscience Journal of Molecular Graphics and Modeling (2009-2011). (xx) He was a Recipient of Chemical Research Society of India Bronze Medal for contributions to Research in Chemistry, 2000 and (xxi) 2014 IBM Faculty Award. (xxii) He was Recognized as one of the top five bioinformaticians in the country (https://bioinformaticsreview.com/awards2018/), (xxii)He was Chairman, DBT Bioinformatics National Certification (BINC exam), 2018. (xxiii) Prof. BJ served as a Referee for several international journals over the years. Prof. Jayaram, published over 150 papers in peer-reviewed international journals, delivered over 300 invited talks (Google Scholar ID: https://scholar.google.com/citations?user=TK_7VNIAAAAJ&hl=en&oi=ao&ORCID/0000-0002-5495-2213).(xxiv) Prof. BJ guided 30 PhD students (27 completed and 3 in progress) and dissertations of several M. Tech. and M.Sc. students. (xxv) Prof. Jayaram is responsible for the creation of science and software of *Chemgenome*, the genome annotation software, *Bhageerath*, the protein structure prediction websuite, *Sanjeevini*, the computer aided drug design software suite, the *Dhanvantari* (Genome→Drug pathway) suiteand several other molecular modelling and bioinformatics utilities, and (xxvi) making these software tools freely accessible to the global user community through scfbio website (www.scfbio-iitd.res.in). (xxvii) Prof. Jayaram is currently Mentor, SCFBio, IIT Delhi (2023-2027).

Prof. (Dr.) Deepak Teotia

Prof. (Dr.) Deepak Teotia, has been dynamically involved in teaching and drug discovery research for the last 25 years. He was awarded his Ph. D. degree from the VMU, Chennai in 2015. All through his 25 years of teaching and research experience and 5 years industrial experience, he has 2 patents, more than 50 papers in national and international journals, 15 conference papers in his credit. He has guided a number of 40 students for the award of their master and doctoral work. He was the Co-Chairman of CMTPI-2017 and Chairman of CTPMS 2020. He has excellent expertise for the administration development of 4 pharmacy institutes and he is solely devoted to generate competent candidates for the education excellence.

Prof. Diwan S Rawat, *FNASc, FRSC, CChem (London)*

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 National Institute of Pharmaceutical Education and Research, Mohali and joined Delhi University in 2003. Prof. Rawat has published over 166 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 with Fellow of National Academy of Sciences (2022). He became the third Professor to get this honour from Delhi University Chemistry Department in last 100 years, and second from Uttrakhand to receive this honour in Chemistry, after Prof DS Bhakuni, his PhD supervisor who received this honour in 1977. Vasvik research award (2022),ISCB Excellence award in drug discovery (2022),Excellence Award for Exemplary Services, University of Delhi 2021,Professor SP Hiremath Memorial Award, Indian Council of Chemist (2016),Professor RC Shah Memorial Lecture Award, Indian Science Congress (2015),Associate Editor, Royal Society Advances and Scientific Report.He has held positions such as Vice Chancellor, Kumaun University Nainital (July 2023 – Till Date).,Dean Examinations, University of Delhi, Delhi (2020 – 2023).,Coordinator, M. Tech (CSPT), Department of Chemistry (2010 – 2016).,OSD University Press (2011 – 2016).,Warden and Provost, Jubilee Hall, University of Delhi (2003 – 2019).

Prof. Dr. Dmitry Druzhilovskiy

Currently holding the position of Senior Scientist at the Institute of Biomedical Chemistry (IBMC) in Moscow, Dmitry's work revolves around various aspects of drug discovery and computational biology. He earned his M.Sc. in Medicine from the Medical & Biological Faculty of the Pirogov Russian National Research Medical University, Moscow, in 2005. Subsequently, in 2014, he obtained his Ph.D. in bioinformatics and mathematical biology from the Institute of Biomedical Chemistry, specializing in the search and optimization of properties for new HIV-1 integrase inhibitors using computer-aided drug design techniques. He serves as the senior coordinator for the development and maintenance of the Way2Drug online platform, which predicts spectra of biological activity. He is also deeply involved in developing novel approaches for drug repositioning and has contributed to the creation of a curated World Wide Approved Drugs online database, serving as a gold standard for training sets estimation. Additionally, he leads the development of a Russian global learning platform aimed at training (Q)SAR methods for estimating spectra of biological activities of new chemical compounds. He has played pivotal roles in numerous international projects, collaborating with esteemed institutions such as the National Institutes of Health (NIH) in the USA and various European and Indian research organizations. His research interests span bioinformatics, chemoinformatics, computer-aided drug design, molecular design, and web technology. In recognition of his significant contributions, Dmitry was honored with the Medal "For contribution to the implementation of state policy in the field of scientific and technological development" in 2021. His extensive publication record reflects his dedication to advancing scientific knowledge, particularly in drug discovery and computational biology.

Prof. Dr. Gunda Georg

Prof. Georg earned aB.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 as a professor and founded the Institute for Therapeutics Discovery and Development she directs. In 2018, she was named Regents Professor. She was Head of the Department of Medicinal Chemistry from 2007-2022. ShewasCo-Editor-in-Chief of *The Journal of Medicinal Chemistry*from 2011-2020. She serves asCo-series Editor of *Topics in Medicinal Chemistry* (2008-present). 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 ACS. In 2020, she received the Alfred Burger Award in Medicinal Chemistry from the American Chemical Society.In 2023, she received the Carl Mannich Medal of the German Pharmaceutical Society. Prof. Georg is the co-inventor of Lusedra^{TM}, which was approved by the FDA in December 2008 and marketed by Eisai Pharmaceuticals. Lusedra is a prodrug of the anesthetic propofol. She is a co-inventor of Minnelide, an anticancer agent currently in phase I/II clinical trials. Several clinical trials are ongoing, and patients are being recruited. She is the co-inventor of a glaucoma drug in phase I/II clinical trials and the non-hormonal male contraceptive YCT-529 that entered a Phase 1a clinical trial in December 2023 in the UK. Prof. Georg has advised 50 graduate students, over100 postdocs, and visiting scientists. She has published >250 peer-reviewed manuscripts.

Dr. Gyan Prakash Modi

Dr. Gyan Prakash Modi, after finishing the course work for a master's degree from IT(BHU), moved to CDRI, Lucknow, to carry out a research project under the supervision of Dr. Anil K Saxena. He finished PhD from Wayne State University, USA, in 20013. He received two years of postdoctoral training from Brandeis University (2014-2015). He joined dept. of pharmaceutical engineering and technology IIT (BHU) in 2016 as an assistant professor and currently serving as associate professor. His research focuses on the development of novel multifunctional drugs for multifactorial diseases, including Alzheimer's and Diabetes. His laboratory is extensively involved in developing novel therapeutic, diagnostic, and theranostic agents for AD. The exosome-based formation is under development in his laboratory to deliver the lead candidates as late-stage preclinical studies. The projects are funded by SERB and ICMR. He is in receipt of the Frank O. Taylor Award in recognition of outstanding scholarship and academic performance at Wayne State University. He was awarded a graduate research assistantship to pursue a Ph.D. and a Master's degree.

Prof. Dr. Indira Ghosh

Prof. Indira Ghosh is working in JNU since 2008 as Dean & Professor to steer the School ofcomputational & 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 (DBT), Govt. of India (GoI) 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, leaving her corporate job from AstraZeneca in Bangalore. After completion of M.Sc. in Physics from Calcutta University she received in 1982 her PhD at IISc, Bangalore under the guidance of Prof. V.S.R.Rao in Molecular Biophysics, a group lead by G.N.Ramachandran. She joined University of Houston, USA as Fulbright Scholar during 1983-1986 with Prof. J. Andrew McCammon and contributed to novel method in computational Biology. 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, MeITy (Ministry of Electronic Communication & Information Technology) and ICMR respectively. Presently, she is editing/contributing a Book (Springer) on Text mining in Biomedical fields & has been working as Bioinformatics Strategist (2021-) to a Start up named TEORA.

Dr. Indrani Bera

Dr. Bera is a scientific researcher with expertise in bioinformatics, peptidomics and cheminformatics. Currently as Marie Curie fellow at UCD, she is using proteomics and peptidomics to understand the natural shift in proteolytic events of plant seeds and analyzing proteomics data of human serum samples and faecal samples using R and python. She has extensiveexpertise in bioinformatics, computational biophysics and computer-aided drug design. She has expertise inexperimental proteomics and peptidomics. She is skilled in analyzing proteomics and peptidomics data, sequenceanalysis, macromolecular modeling, molecular dynamics simulations and structure- and ligand-based computational drug design. She has proficiency in R,Perl and python scripting. She is author of 17 peer reviewed publications including 9 first authors. Her research goal is to apply my integrated bioinformatics skills to dissect massive biological data at genomic/proteomics level and small molecule level for better understanding of human health. Her other research interests are to understand how various protein sequences influence their structure and function; and to study changes in conformational dynamics of protein facilitating their function at different conditions.

Dr. James Devillers

James Devillers is head of CTIS. His research activity deals with (Q)SAR, QSPR, and (eco)toxicology modeling with a specific focus on the use of nonlinear methods. He has published more than 250 peer-reviewed papers and book chapters and also authored/edited 17 books. J. Devillers is editor-in-chief of the journal *SAR and QSAR in Environmental Research* (Taylor & Francis) and editor of the series of books *QSAR in Environmental and Health Sciences* (CRC Press). He is also member of the editorial boards of *Ecological Modelling* (Elsevier), *Xenobiotica* (Taylor & Francis), and *Toxics* (MDPI - Open Access Publishing). He is at the origin of the CMTPI meetings and he has (co-)organized numerous international conferences in QSAR and drug design.

Prof. Dr. Kuldeep Kumar Roy

Prof. Kuldeep Kumar Roy is a seasoned professional with over 16 years of teaching and research experience at several national and international institutions. Prof. Roy is currently employed at UPES, Dehradun, Uttarakhand, as a Professor and Cluster Head in the Pharmaceutical Sciences cluster, School of Health Sciences and Technology. He earned his Bachelor of Pharmacy (B.Pharm.) and Master of Pharmacy (M.Pharm.) in Pharmaceutical Chemistry degrees from Birla Institute of Technology in Mesra (Ranchi), Jharkhand. He received his Doctor of Philosophy (Ph.D.) in Medicinal Chemistry under the supervision of Prof. Anil Kumar Saxena from the CSIR-Central Drug Research Institute in Lucknow and the Jawaharlal Nehru University (JNU) in New Delhi, India, jointly. He spent several years doing post-doctoral research in South Korea and the United States. He specialises in Pharmaceutical Research, Bioinformatics, Medicinal Chemistry, and New Drug Discovery, among other things. He has interest in translational drug discovery research for diseases of unmet need through the integration of computational modeling and medicinal chemistry. He has received funding support from several government bodies, including the ICMR, CSIR, DST, and DBT. He has three international patents (granted) and over 45 peer-reviewed international publications to his credit. He has attained H-index of 19 and i10-index of 29 till date.He is currently serving as an Associate Editor in the Frontiers in Drug Discovery journal. He has served as reviewer of several international journals.

Prof. Dr. Kunal K.Ganguly

Kunal K.Ganguly is a faculty in the area of Operations Management and Decision Science with the Indian Institute of Management, Kashipur. He has done his master's degree and Ph.D. from IIT Kharagpur. He has more than two decades of experience in academics. He has publications in many reputed international journals. His areas of interest are Supply Chain Management and Quality management. He also has more than six years of experience in the industry in various fields of Operation, Quality Control, and Training.

Dr. Marjan Vračko 

Dr. Marjan Vračko is senior researcher at Kemijski Inštitut/National Institute of Chemistry in Ljubljana, Slovenia. Since 1994 his research is focused to QSAR (quantitative structure-activity relationship) modelling of biological/toxical properties of compounds, to quantum chemistry, to chemometrics (numerical analysis of proteomic and genomic data) and to modeling of interaction between receptors and molecules. He obtained his PhD (1990) under supervision of Prof. Janos Ladik from University of Erlangen, FR Germany in the field of quantum chemistry. Later on he was post doc at the Columbia University of New York and at the University of Namur, BE (Faculté Universitaire Notre Dame de la Paix, Namur). In 1994 he joined the National Institute of Chemistry in Ljubljana. In 2005 he was senior visiting researcher at the Joint Research Centre of European Commission, Ispra where he worked on applications of (Q)SAR methods for regulatory purposes. He is author of 90 scientific papers and several chapters (Hirsch index h = 31). From 2000 to 2023 he supervised three doctoral candidates and six post doctoral researches, who proceed their careers in Academia and in multinational companies (Nestle, KNÖLL GmbH, SPM AG Liechtenstein).

Dr. Madhumita Dandopath Patra 

Dr. Madhumita Dandopath Patra graduated from the Bankura Christian college and secured first place amongst all streams of the college and won Sachhidananda Gold Medal, 2000, P.C .Roy memorial scholarship, 2000 and the National Scholarship, 2000. She did my post graduation in Chemistry with Organic chemistry as a special paper, from University of Burdwan , 2002. She won the Bronze medal for achieving highest marks in Organic Chemistry,2002. After qualifying for UGC -CSIR NET, She completed Ph.D. from Indian Institute of Chemical Biology (IICB), 2008, Kolkata. Then she took an attempt for DBT Post doctoral research fellowship, and qualified for the same, did my Post doctoral research in the field of " Protein crystallography" from Saha Institute of Nuclear Physics in 2009. In 2010, she appointed as an Assistant Professor in the Dept of Chemistry , Acharya Prafulla Chandra College, under West Bengal State University. Her research work in the field of Structural Biology and Theoretical Chemistry. Her passion for research in science helped to publish 11 research papers with 9 of them as lead author, in reputed International journals and she presented my work in several International and National seminars. She is experienced with software development, it comes naturally to encourage my students to use different technological tools. She has been performing a lots of administrative work in my college.

Mr. Naveen P Deshpande 

Mr. Naveen Pralhad Deshpande is a seasoned entrepreneur and a globally recognized executive in the software industry. With a track record of cofounding three successful software technology start-ups over the past 16 years, he currently serves as the Co founder and Group Chief Operating Officer at entomo. Naveen is a highly sought-after keynote speaker and panellist at software technology industry events, where he shares his expertise on digital transformation in the public sector and enterprises. Naveen is an angel investor and a venture partner with Vickers Venture Partners, a globally renowned deep tech venture fund, where he contributes in identifying and supporting promising start-ups in the technology sector. Naveen holds a distinguished engineering degree and a prestigious global MBA, earning the honour of a gold medal for his outstanding academic achievements.

Prof. Om Prakash 

Dr. Om Prakash**,** is a full professor of Biochemistry and Molecular Biophysics (BMB)and Chair, BMB Graduate Program admission at Kansas State University (KSU), Manhattan, KS, USA. He joined KSU in 1993 after doctoral training at the medicinal chemistry division of Central Drug Research Institute (CDRI), Lucknow, India, postdoctoral trainings at Stevens Institute of Technology, Hoboken, NJ and at University of Arizona, Tucson, AZ. He also directs Mary L. Vanier Biomolecular NMR Center at KSU and his laboratory research has been focusing on the structure, function and molecular recognition using Nuclear Magnetic Resonance (NMR) and NMR structure-based drug designing.

Dr. Omer Saka

Dr Omer Saka is a medical doctor with expertise in the field of health economics and business development. After his graduation in medicine from Istanbul, Turkey, Dr Saka pursued higher studies in health policy, planning and financing from the prestigious London School of Economics and Political Science (LSE). He is known for his business acumen and skills in health economics modelling. Dr Saka has pivoted in establishing life science and health consulting in Big4s and has excelled in to position of partner in the global business world. He is associated with major pharmaceutical companies and public health institutions as an external expert and consultant to various projects related to clinical observational studies, health economics evaluation, AI-driven systematic literature reviews and patient care in the fields of cardiovascular, endocrinology and infectious diseases.

Dr Saka continues to serve the life sciences sector in his role at high managerial levels and would enrich the symposium with his management and business development skills.

Prof. Dr. P.V. Bharatam

Prof. Bharatam is currently a Professor and Head in Department of Medicinal Chemistry in National Institute of Pharmaceutical Education and Research (NIPER), Mohali. His field of specialization includes Medicinal Chemistry, Theoretical Organic Chemistry, Organic Synthesis, Molecular Modeling and Pharmacoinformatics. Prof. Bharatam completed his Ph.D. in 1990 from Univ. of Hyderabad, India in Applied Theoretical Chemistry. He has a total of40years research experience which includes 4 years in USA and Germany and 27 years of teaching experience. Apart from his current position he had held various positions such as Assoc. Dean (Academics) during 2015-2016 and Dean, NIPER, SAS Nagar during 2016-2018. He is the recipient of various awards such as OPPI Scientist Award in Medicinal Chemistry in 2009, Ranbaxy Research Award in Pharmaceutical Sciences in 2008, Chem. Research Society of India – Medal in 2008, Fellowship of Royal Society of Chemistry, London in 2007, IBM Faculty Award in
2007 and Fellowship of Alexander von Humboldt Stiftung, Bonn in 2002 etc. Till now he has supervised more than 36 Ph. D. students, 173 M.S. Pharm. students, 16 M. Sc. Chem. Students and 12 Fellows. He has received 15 Govt. funded projects, 6 Institutional grants and 2 Industrial grants. Prof. Bharatam has more than 265 Original Scientific articles (non-Indian journals), 19 Original Scientific articles (Indian Journals), 23 Reviews (peer reviewed) and Book Chapters (peer reviewed) and 15 Science Education articles to his name.

Dr. Rahul Singhal, MD, DNB, FACC(USA), FSCAI(USA),MNAMS

Dr. Singhal is honorable Director of cardiology and cardiac electrophysiology, fortis escorts hospital, jaipur . Dr. Singhal is specialized in Cardiac Arrhythmias and Pacing and Heart Failure management, with vast experience of 16 years in field of Cardiology and Cardiac Electrophysiology. He is Well versed in all elective and complex Coronary, peripheral and structural Cardiac Interventions like calcified lesions with ROTA ablations, IVL, IVUS and OCT. He performed TAVI and multiple Conduction system pacing and leadless pacemakers (MICRA). He had Post doctoral degree from Escorts Heart Institute, New Delhi. He achieved prestigious Fellowship in Cardiac Electrophysiology at Taipei, Taiwan under guidance of world-renowned Cardiac Electrophysiologist Dr. Shih Ann Chen. He had Publications in various National and International journals. He Represented India at various International Conferences. Dr. Singhal has been awarded "Best Cardiologist in Rajasthan Award" for 2 consecutive years presented by Health Minister and Sunil Gavaskar. Has performed over 6500+ Pacemakers; 1500+ ICDs; 1000+ CRT's; 5000+ EPS and RFA's and nearly 20000+ Coronary and Peripheral Interventions so far. He is the sub committee member ,clinical research, asia pacific heart rhythm society (APHRS) Executive member CSI (RAJASTHAN), IHRS, CSI.

Dr. Sanjay Batra

Dr. Sanjay Batra completed his Ph.D. in 1993 from the Medicinal and Process Chemistry Division at Central Drug Research Institute, Lucknow. He joined as faculty in the same department in 1995 and is presently working as a Chief Scientist and head of the department. Between November 2000 and November 2001, he worked as a visiting scientist at the Chemistry Department, University of Mississippi, Oxford. He has made significant contributions tomedicinal and organic chemistry with special emphasis on developing new drugs for neglected diseases. Two molecules one each for treating Visceral Leishmaniasis and Neuropathic pain (biased KOR agonist) from his research group are undergoing advanced IND enabling studies. He has also contributed to obtaining the IND permission to conduct clinical trials of a new antithrombotic compound licensed to the industry in 2021. He has more than 150 research publications, 17 review articles,8 patent applications, and 3 book chapters to his credit. 21 students have completed PhD under his supervision. His research interests include the development of chemistry associated with Morita-Baylis-Hillman adducts, transition metal and iodine-catalyzed reactions, and heterocyclic chemistry. He is a fellow of the Indian National Science Academy and a Fellow of the Royal Society of Chemistry. He is the recipient of a Bronze medal from the Chemical Research Society of India (CRSI). He is a member of the International Advisory Board of *ChemMedChem* (Wileys publication). He has earlier served as Associate Editor for RSC Advances (2015-2017) and Chief Editor of Anti-Infective Agents (Bentham Publications (2011-2017). He is a member of the PAC-CRG-SERB, Organic Chemistry and PAC-SRG & nPDF, SERB, Biological Sciences. He has beena member of the SERB-Covid task force too since it was constituted.

Prof. 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

Dr. Sisir Nandi is working as Professor and Head, Global Institute of Pharmaceutical Education and Research, Kashipur. He is the Organizing Secretary of this symposium. Dr. Sisir Nandi completed Ph.D. from Indian Institute of Chemical Biology (CSIR), Kolkata as a CSIR - GATE fellow 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 fellowship in Laboratory of Chemometrics, National Institute of Chemistry, Ljubljana, Slovenia, Europe. Dr. Nandi is working in the area of anti-COVID-19, anticancer, antiviral, antitubercular, antimalarial drug design, development and discovery research. He published more than 110 original research articles and reviews in reputed international journals having high impact factor. He published 6 book chapters in SpringerNature and Bentham book. He has H-index of 15. He presented his research work in many international conferences round the globe. He is Guest Editors of Current Signal Transduction Therapy and Current Pharmaceutical Design. He is having more than 15 years of teaching and 18 years of research experiences. He has been guiding many masters and doctoral students. He is very competent in organizing many Govt funded international seminar, conferences and symposia as organizing Secretary.

Prof. Dr. Soniya Nityanand

Prof. Dr. Soniya Nityanand, honorable Vice Chancellor of King George Medical University, Lucknow, is an immunologist specialising 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, Sweden in 1996.

She served as Prof and Head, Dept. of Hematology and Stem Cell Research Centre, SGPGIMS, Lucknow from 2003 to 2021. She was Executive Registrar, SGPGIMS, Lucknow (Additional Charge) from 2018 to 2021, Chief Medical Superintendent, SGPGIMS, Lucknow (Additional Charge) Feb 2021-May 2021. She is honorable Vice Chancellor, King George's Medical University, Lucknow from August 09, 2023 – till date and Director, Dr Ram Manohar Lohia Institute of Medical Sciences, Lucknow fromMay 2021- till date.

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 and Chancellor's Medal for the best Medical Student.

Dr. Subhash C. Basak

Dr. Subhash C. Basak is a retired Adjunct Professor in the Department of Chemistry and Biochemistry, University of Minnesota Duluth, USA. He received his PhD in biochemistry in 1981 from the univeristy of Calcutta, India. His currentresearech intterests involve discrete mathematical chemistry and its applications to chemoinformatics,bioinformatics, quantitative structure-activity relationship (QSAR), computaational toxicology,mathematical quantification of DNA/ RNA sequences, mathematical proteomics,and computer-aided vaccien design for emerging pathogens like Zika virus, COVID-19. Dr. Basak is the fromer Editor-in-chief of rthe itnernatioanl journal Current Computer Aided Drug Design. He was involved in editing four books: 1) Statistical and Machine Learning Approaches for Network Analysis, Wiley, 2012; 2)Advances in Mathematical Chemistry and Applications, Volume 1 & 2, Elsevier & Bentham Science Publishers, 2015; 3)Zikavirus: Basic biology, surveillance, vaccine design and anti-Zika drug discovery: Computer-assisted strategies to combat the menace, Nova ,2019 and 4) Big Data Analytics in Chemoinformatics and Bioinformatics: With Applications to Computer-Aided Drug Design, Cancer Biology, Emerging Pathogens and Computational Toxicology. Dr. Basak has authored more than 350papers and book chapters (https://www.researchgate.net/profile/Subhash-Basak). He received a total of US $7,466,017 in grants and contracts. He is the past President of the internaitonal society of mathematical chemistyr and a member of the internatinal academy of mathematical chemisty (IAMC). He is the foiunder Chairperson of three mathematical chemistry conference series involving India, USA and countries of South America.

Dr. R. Natarajan

Dr. R. Natarajan Completed M.Sc. in chemistry in 1979 from St Joseph's College, Tiruchirappalli, Tamil Nadu affiliated to Madras University. Started his carrier as a chemistry teacher for Grade 11 and 12 and then pursued M.Phil. in Chemistry from Bharathidasan University, Tiruchirappalli, Tamil Nadu in 1988. The M.Phil. thesis results were presented in the American Chemical Society meeting held in Toronto, Canada in 1988. Continued to complete Ph.D. in chemistry from Bharathidasan University, Tiruchirappalli, Tamil Naduin the year 1995. Part of the Ph.D. research was carried out in Chemical Engineering Department, Lakehead University, Thunder Bay, Canada. Visited Lakehead University, Canada four times in 1995, 2000, 2002-04, 2007-09 as visiting faculty, research associate and exchange visitor. From 2004-07 worked as a Scientist in Dr Subhash Basak's groupat Natural Resource Research Institute, Duluth, Minnesota, USA.From 2010 to 2019 worked as the CEO of a polymer company in Karur, Tamil Nadu. During this period 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.

Dr. Yusra Ahmad

Dr. Yusra Ahmad is a distinguished academician, possessing a robust academic background and technical expertise in the field of pharmacology. She holds a Ph.D. in Medical Pharmacology from the prestigious Department of Pharmacology, Faculty of Medical Science, Delhi University, in collaboration with the Department of Biochemistry, All India Institute of Medical Sciences (AIIMS, Delhi). Her academic journey also includes an M.Pharm in Pharmacology from Jamia Hamdard, New Delhi, and B.Pharm from Birla Institute of Technology, Mesra, Ranchi. Throughout her career, she has demonstrated a remarkable track record of conducting innovative research and contributing significantly to the advancement of medical science. Dr. Ahmad's contributions extend beyond the confines of the laboratory, as evidenced by her numerous publications in various esteemed national and international journals and book chapters in Science Direct. She is deeply committed to fostering a culture of excellence and innovation across all spheres of her work. Currently, Dr. Yusra Ahmad serves as the Head of the Faculty of Pharmacy at Veer Madho Singh Bhandari, Uttarakhand Technical University. In this capacity, she continues to inspire and guide the academic community towards achieving new heights of excellence in pharmacy education and research.

INVITED LECTURES

Quantitative Structure Interaction Activity Relationship (QSIAR): a novel approach to drug design: a case study of anti-tubercular agent

Anil K. Saxena

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Computer aided drug-design (CADD) an effective tool in the process of drug design and discoveryconsists of ligand-based drug design (LBDD) and structure-based drug design (SBDD). The SBDD has gained importance in recent years due to the developments in molecular biology including genomics, proteomics, and structural informationof new targets.Docking scores play a key role in analysing the results in terms of interactions between the structural components of the interacting molecule with the target protein. The docking scores generally do not correlate with the observed biological activity. This may be attributed to the limitations in scoring functions used in docking algorithms which often fail to account for crucial factors like entropy change, solvation effects, and interactions, contributing to binding affinity limiting the accurate prediction of binding energy changes, which may resultin the poor correlations between observed biological activity and docking scoring functions.In this context, a maiden novel approach (Quantitative Structure Interaction Activity Relationship (QSIAR)) has been applied to address this issue bytaking into account the specific interactionsbetween a ligand and the amino acid residues present at the active siteas independent and biological activity as dependent parameter(s) inquantitative terms to explain the observed anti-tubercular activity as mycobacterium ATP synthase inhibitory activity in diverse molecules such as4-substituted amino sulphonyl-2-methyl-7-chloroquinolines, bisquinoline, imidazo[1,2-a]pyridine ethers and squaramides. The developed and validated quantitative model(s) have led to the identification of novel leads through virtual screening of the focussed libraries for the development of new anti-tubercular agents.

Keywords: Tuberculosis, ATP synthase, QSIAR, virtual screening, SBDD

ONCORx: A digital App for cancer treatment planning

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Purpose: Treatment for breast cancer patients usually comprises multiple modalities, (e.g. surgery, radiation therapy, chemotherapy, hormonal therapy, targeted therapy, bisphosphonates, immunotherapy). Treatments are used at varying frequencies, durations, in combination or sequence, and over an extended period. At initial consultation, patients are presented with new and unfamiliar information on diagnosis and prognosis. Communicating an adaptive neoadjuvant, adjuvant or palliative treatment plan in this environment, together with potential options is challenging for oncologists and often overwhelming for patients. Patients' lack of understanding of the proposed treatment can compromise informed choice, consent, and compliance. To simplify the process ONCORx has been developed.

Methods: The MIRO web interface was used to develop the flow charts for web tool design. Flow charts were based on local treatment protocols /NICE guidelines.

A web application was developed in flutter-based technology. DART language-based programming was conducted to develop the logical framework based on the MIRO decision tree.

Web application development with the option of two user logins: one for a user and another for Admin to enable flexibility/future-proofing as further treatment regimens.

Results: OncoRx App allows oncologists to select relevant treatments according to the patient's breast cancer phenotype and display a simple illustration/flow chart of their proposed treatment plan along with a treatment sequence timeline. The final output offers editing options in both Word and PDF format to share with the patient.

Conclusion: Considering rapid innovation in oncology, especially with an increase in the number of treatment lines, this user-friendly app will help oncologists communicate treatment plans to patients with a timeline to avoid patients missing appointmentsand make things simple for patient to understand.

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Green- and Click-Chemistry:An Opportunity for Simplification and Innovation Towards Natural and Nature-inspired Synthetic Small Molecules of Biological and Commercial Importance

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The concept of green chemistry has a more than twenty-five-year history of invention and innovation of creating new transformations, new products, new manufacturing processes that perform better with less waste and less cost while being sustainable and safe for humans and the environment. Similarly, click chemistry has become known as a fast, selective, wide in scope, efficient, reliable, simple to perform to the synthesis of novel and bioactive compounds inhigh yield with good atom economyand desired functionalities. Thus, the range of products and processes invented and improved by green chemistry and click chemistry touchvirtually every industry sector from medicine to agriculture to energy to plastics to nanotechnology to electronics to polymer to natural products. Small molecules of natural origin including polyphenolics and thiophenol based bioactive compounds have drawn great interest from the scientific community as they are associated with wide range of biological activities including anticancer, antimalarial,antibacterial, antifungal and anti-inflammatory etc. However, exploration of these natural bioactive molecules is severely hindered by their insufficient percentage in their natural resources, difficult isolation procedure, limiting trials for wider applications besides their tedious multistep synthesis involving protection-deprotection strategy. The shortcomings of the prevalent methodologies have provided a fresh stimulus to develop newstrategies based on "Green"and Click Chemistry. Our groups from noticeable time have been working on such green methodologies for extraction and purification of natural molecules as well as design and synthesis of various polyphenolic and thiophenolicbased bioactive molecules like FEMA-GRAS approved 4-vinylphenols, stilbenoids (e.g.resveratrol, Pterostilbene), hybrid molecules (e.gsalvianolic acid F) and 3-sulphenylated indole derivativeswith their biological evaluation. Moreover, the details of microwave- and ionic liquid-promoted step-economical synthesis of such natural and non-natural moleculesofbiological and commercial importance will be discussed during presentation.

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Technology Life Cycle – Concept to Commissioning

Alok Kumar Saxena

Technology Consultant

The ultimate aspiration of every scientist or inventor is to witness their creation playing a pivotal role in the lives of the masses, impacting the environment positively, and serving not only the nation's interests but also global well-being. The journey of innovation begins with conceptualization, traverses numerous stages, and culminates in the development of a technology that can seamlessly integrate into the fabric of humanity's needs. However, for a technology to truly make a difference, it must also be commercially viable.

This presentation delves into the intricate process that any technology undergoes before achieving widespread commercial adoption. The journey involves a combination of time-consuming and investment-intensive steps, collectively shaping the characteristic 'S' curve associated with the maturation of any process. Throughout the presentation, these steps on the 'S' curve are elucidated, shedding light on the inherent challenges associated with technology scale-up and development, as well as emphasizing the crucial aspect of long-term sustainability.

Ritonavir enhances the efficacy of amprenavir in combination in clinically isolated Leishmania parasites

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Visceral leishmaniasis (VL) is the 2nd deadliest parasitic disease in the world caused by unicellular protozoan parasite *Leishmania donovani*. They are transmitted through infected female Phlebotomus sand flies which feed on blood. VL is considered as a Neglected Tropical Disease (NTD) affecting the low-income nations of Asia and Africa and is mainly concentrated in Indian subcontinent. It causes a death toll of 20-30 thousand annually. People from economically weaker sections are generally more prone to *Leishmania* infection, due to their weaker immune system. Ironically, drugs that are in clinical uses against leishmaniasis are very expensive and toxic. There is also an increased incidence of resistance against conventional drugs. Due to these reasons, there is a need for development of new drugs for the treatment of visceral leishmaniasis,which is affordable, non-toxic and effective against those parasites that are resistant to conventional drugs.Moreover, HIV-VL co-infection challenges the control and elimination of VL. So, better alternatives for the treatment of HIV-VL coinfection is urgent need. Therefore, the present study focused on the combinational therapy of HIV-1 protease inhibitoramprenavir in combination with ritonavir inmitochondria-mediated cell death process of *Leishmania donovani*. This combination effectively kills the parasites by targeting *Leishmania* DNA topoisomerase I (LdTopILS) at a lower dose and exerted programmed cell death by increased ROS followed by loss of mitochondrial membrane potential, caspase activation and DNA fragmentation.Therefore, the study might be exploited for the therapeutic development against HIV-VL coinfectionas well as a substitute to replace the conventional drugs.

Identification of targeted therapeutics against oral squamous cell carcinoma

Anshuman Dixit

Institute of Life Sciences,Bhubaneswar

Oral cancer with about 80000 cases/year is a big concern in India. Majority of the oral cancer cases are oral squamous cell carcinoma (OSCC). Consumption of alcohol, chewing tobacco, areca nut, and smoking are significant risk factors associated with oral cancer. Major problems associated with oral cancer treatment are unavailability of targeted therapies and development of chemoresistance.To address the challenge, we devised a bioinformatics pipeline using gene expression analysis, Cox proportional hazard regression, and machine learning to identify genes that can stratify the OSCC patients by risk profile (high-low). We also analyzed the identified genes (BOP1, CCNA2, CKS2, PLAU, and SERPINE1) for their involvement in other cancers as well as in chemoresistance in multiple cancer cell lines.

It is pertinent to note there are no drugs available against these biomarkers to date. Therefore, a comprehensive in silico drug design strategy assimilating homology modeling, extensive molecular dynamics (MD) simulation and ensemble molecular docking has been applied to identify potential compounds against identified targets, and potential molecules have been identified. We hope that this study will help in deciphering potential genes having roles in chemoresistance and a significant impact on OS. It will also result in the identification of new targeted therapeutics against OSCC.

Strategic Formulation And Evaluation Of Nano-Insulin In Combating Arsenic-Induced Hyperglycemia In Mice Model

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Diabetes is a menacing problem,affecting millions of people globally. Inhabitants of groundwater arsenic contaminated areas suffer from hyperglycemia leading to diabetes and its complication. Insulin is used by mass to combat diabetes trailing with incidences of drug resistance and drug dependence as the usual setback entailing the need for designing new advanced drug to address the issue. The present studyevaluates whether PLGA-loaded nano-insulin (NIn) has a greater cost-effective anti-hyperglycemic potential than that of insulin in chronically arsenite-fed diabetic mice. The particle size, zeta potential of NInwas determined by AFM, DLS. The ability of NIn to cross the blood–brain barrier (BBB) was also checked. Circular dichroic spectra (CD) of insulin and NIn in presence/ absence of arsenic were compared. Diabetic markers,mitochondrial functioning through indices like Cytc, pyruvate-kinase, glucokinase, ATP/ADP ratio, MMP, CMP and Ca^{2+} level were evaluatedin different mice groups. Expressions of the relevant marker proteins and mRNAs like insulin, GLUT2, GLUT4, IRS1, IRS2, PI3, bcl2, caspase3 for tracking-down the signaling cascade were also analyzed. Results revealed that NIn, due to its smaller size, faster mobility, site-specific release, could cross BBB and showed positive modulation in mitochondrial signaling cascades and other downstream signaling molecules in reducing arsenic-induced-hyperglycemia. CD data indicated that NIn had less distorted secondary structure as compared to insulin in presence of arsenic. Thus, overall analyses revealed that PLGANInshowed better efficacy in combating arsenite-induced-hyperglycemia than that of insulin and therefore, has greater potentials and possibility for usage in future clinical trials.

Keywords: Nano-insulin (NIn), arsenic, blood-brain-barrier, signalling cascade, mice

Pyrazolo[4,3-c]pyridine Sulfonamides as Carbonic Anhydrase Inhibitors: Synthesis, Biological and In Silico Studies

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Carbonic anhydrases (CAs, EC 4.2.1.1) catalyze the essential reaction of CO_2 hydration in all living organisms, being actively involved in the regulation of a plethora of patho-/physiological conditions. A series of chromene-based sulfonamides were synthesized and tested as possible CA inhibitors. On the other hand, in microorganisms, the β- and γ- classes are expressed in addition to the α- class, showing substantial structural differences to the human isoforms. In this scenario, not only human but also bacterial CAs are of particular interest as new antibacterial agents with an alternative mechanism of action for fighting the emerging problem of extensive drug resistance afflicting most countries worldwide. Pyrazolo[4,3-c]pyridine sulfonamides were synthesized using methods of organic chemistry. Their inhibitory activity, assessed against the cytosolic human isoforms hCA I andhCA II, the transmembrane hCA IX and XII, and β- and γ-CAsfrom three different bacterial strains, was evaluated by a stopped-flow CO_2 hydrase assay. Several of the investigated derivatives showed interesting inhibition activity towards the cytosolic associate isoforms hCA I and hCA II, as well as the 3β- and 3γ-CAs. Furthermore, computational procedures were used to investigate the binding mode of this class of compounds within the active site of hCA IX. Four compounds (**1f**, **1g**, **1h,** and **1k**) were more potent than AAZ against hCA I. Furthermore, compound **1f** also showed better activity than AAZ against the hCA II isoform. Moreover, ten compounds out of eleven appeared to be very potent against the γ-CA from *E.coli,* with a Ki much lower than that of the reference drug. Most of the compounds showed better activity than AAZ against hCA I as well as the γ-CA from *E.coli*and the β-CA from *Burkholderiapseudomallei (BpsCAβ).* Compounds **1f** and **1k**showed a good selectivity index against hCA I and hCA XII, while **1b** was selective against all 3β-CA isoforms from *E.coli*,*BpsCA*,and *VhCA*and all 3γ-CA isoforms from *E.coli*,*BpsCA*,and *PgiCA.*

QUANTUM COMPUTING MACHINE LEARNING FOR DRUG DISCOVERY

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Quantum computing and machine learning are poised to revolutionize drug discovery, offering novel approaches to address the complexities of identifying and developing new therapeutics. Quantum computing harnesses the principles of quantum mechanics to perform computations exponentially faster than classical computers, opening avenues for simulating molecular interactions and predicting drug-target binding with unprecedented precision.At its core, quantum computing leverages the principles of quantum mechanics to process information in ways that far exceed the capabilities of classical computers. In the realm of drug discovery, this translates into the ability to simulate and analyse molecular structures and interactions with unprecedented accuracy and efficiency. By harnessing the unique properties of quantum systems, such as superposition and entanglement, quantum computers can explore vast chemical spaces, predict molecular properties, and elucidate intricate biochemical pathways that underpin disease mechanisms.Machine learning complements this by analysing vast datasets of molecular structures, biological pathways, and clinical data to uncover patterns and relationships that guide drug discovery efforts.One of the most promising applications of quantum computing and machine learning in drug discovery is the optimization of molecular structures. Quantum algorithms can efficiently explore the vast chemical space to identify lead compounds with desirable properties, while machine learning models can predict the bioactivity and pharmacokinetic profiles of these compounds, accelerating the process of drug candidate selection. Other exciting areas where Quantum Machine Learning can enable are Molecular Property Prediction, Molecular Docking and Binding Affinity Prediction, Drug Repurposing and Multi-Modal Data Integration, Adverse Drug Reaction Prediction and Drug Safety Assessment and more.

Visible-Light-Mediated Synthesis of Functionalized Heterocycles

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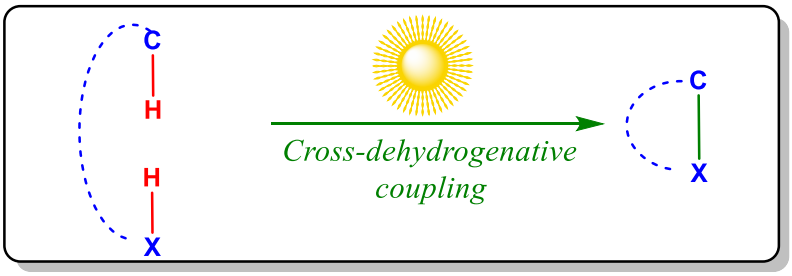
Heterocycles are the core structure of the majority of commercially available pharmaceuticals. As a consequence, synthetic chemists have paid attention to the development of new synthetic methodologies for the synthesis of functionalized heterocycles over the years. On the other hand, designing a methodology through a green pathway is highly desirable for sustainable development. So, developing synthetic strategies towards functionalized heterocycles through atom-, time-, step- and cost-effective pathways is one of the important areas of research. Cross-dehydrogenative coupling offers all of these advantages and has gained the interest of chemists.[1] If this green strategy could be carried out with visible light as the energy resources it would also add another feature i.e. energy efficiency.[2-3] So, we are interested in investigating on the designing and synthesis of visible-light-induced synthesis of functionalized heterocycles from easily accessible reactants *via* cross-dehydrogenative coupling reactions. I will discuss our findings in this field for the synthesis of functionalized fused furan and pyrazole derivatives.[4-6]



Scheme 1: Organophotocatalyzed cross-dehydrogenative coupling.

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The Many Facets of AI/ML along Genome to Drug Pathway

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Some, major steps along the Genome to Drug pathway involve genome annotation, target protein's structure prediction, active site identification, virtual screening of small molecules against the target protein, docking and scoring potential inhibitor molecules for further experimental validation. Here, we trace the evolution of AI/ML methods along this pathway highlighting some contemporary strategies for an effective prediction of promising candidate drug molecules.

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

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

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WAY2DRUG: EFFICIENT PREDICTION OF BIOLOGICAL ACTIVITIES FROM GLOBAL TO LOCAL SCALES

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Global chemical space is extremely vast and finding a molecule with the required pharmacotherapeutic property is a formidable challenge.Starting from analysis of big chemical-biological data obtained*in silico, in vitro, in vivo* and *in clinics* it is necessary to finish with one active pharmaceutical ingredient possessing the needed safety and efficacy.Combining information extracted from thecurated datasets of active/inactivecompoundsavailable via World Wide Web with computational AI/ML tools investigators are surfing from global to local scales in pharmaceutical R&D,enabling faster and more efficient development of new therapeutic remedies.

Way2Drug (https://www.way2drug.com) is a quickly expanding web portal focused at integrating of demanded in silico tools for drug discovery. Way2Drug currently hosts services for predicting the biological activities (PHARMA), toxicity (TOX), metabolism (META) and physicochemical characteristics (ADME) of drug-like molecules. All tools are freely available for non-commercial academic research.

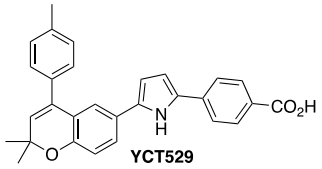
Way2Drug is evolving as the basis for development of computational platform for efficient analysis and interpretation of the extensive biomedical and clinical data, comparative analysis of information extracted from these data to differentiate the normal and pathological states, obtaining new knowledge to identify potential pharmacological targets and biomarkers, designing potential pharmacological substances with the required properties, determining the optimal approach to therapy taking into account the individuality of patients.

The study is performed in the framework of the Program for Basic Research in the Russian Federation for a long-term period (2021-2030) (No. 122030100170-5).

The Male Pill: Are We There Yet?

Gunda Georg, USA

To provide couples with additional safe and reversible options for contraception, the development of non-hormonal contraceptives for both men and women is highly desirable to assist with family planning and reducing unintended pregnancies. The talk will provide an overview of the current state of hormonal and non-hormonal male contraceptive drug discovery and development with an emphasis on the discovery and development of retinoic acid receptor alpha antagonists, including preclinical efficacy studies of our preclinical candidate YCT529 in mouse and non-human primates. YCT529 entered a Phase 1a clinical trial in December 2023.



YCT529

	α	β	γ
IC_{50} (nM)	9.7	> 3500	>35000
	no agonist activity		

Development of naturaltemplate-based novel diagnostic and theranostic agents and their formulation development for Alzheimer's disease

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Alzheimer's disease (AD) is a brain related neurological disorder characterized by gradual loss in memory along with other peripheral and central symptoms. The currently available treatments for AD provide only symptomatic relief without addressing the pathological hallmarks of the disease, therefore, neurodegeneration continues with these therapies[1]. Natural products have gained enormous interest in preventing or diagnosis of AD. Intriguingly, these natural products also suffer from several drawback and not druggable[2]. To address the issues associated with natural products, we developed ferulic acid (FA) and rivastigmine analogs as therapeutic and theranostic agents for AD.

Naturally inspired novel molecules were designed, synthesized and characterized following the art of medicinal chemistry. The enzyme inhibition studies were carried out with modified Ellman method[3]. SH-SY5Y cells were utilized to evaluate the neuroprotection ability of the lead moleculesThe *in-vivo* studies were carried out in various AD mice, drosophila models and in AD autopsy samples.

The lead molecules were found to be potent inhibitors of AChE/BChE (IC_{50}= 0.79±0.1nM, and 3.97±0.8nM for BChE and AChE, respectively).The lead molecules exhibited promising antioxidant, $A\beta_{1-42}$ and tau aggregation modulation, NLRP3 inhibition, and metal chelation property. Further, the lead molecules were efficacious in the AD drosophila model, *in-vivo* and ex-vivo in scopolamine-induced AD models.

The development of another series of diagnostic and theranostic probes is also inspired on nature product. The lead probe molecules have shown promising and selective Aβ aggregation detection ability in different AD models including transgenic AD mice model and AD patient autopsy samples.The unique ocular imaging pattern in the AD Drosophila model, strongly suggest that probes hold promise as a dependable indicator for rapid, noninvasive assessment of new therapeutic modulators or inhibitors in AD.

We are developing the exosome-based formulation of the lead identified in our laboratory.

Acknowledgment: GM is thankful to the Science and Engineering Research Board under Core Research Grant (SERB-CRG/2018/003490), the Indian Council of Medical Research(ICMR/EMR/2019-3088),(ICMR/ EMR/2021-10363). GM also thanks Dr. Anita Mahadevan, Coordinator, Human Brain Bank (NIMHANS), for providing the autopsy tissue samples from clinically diagnosed AD patients.

Strategy to Combat Persistent Tuberculosis: Entrapment of Flow of Substrate in Non-Essential Pathway

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The post genomic era has provided the leap into the hypothesis based biology in the field of the "omes" & "omics" world. Designing of drugs are no longer contained in the domain of physiology & medicinal chemistry, process changed other way, for biologists it is utmost important to know the cause & mechanism of disease, relevance of balancing the flow of substrate & inhibitor etc in the metabolism of systems. But The importance of reorganizing our thinking process is mostly reflected in the merger & acquisition of Biotechnology, Bioinformatics and Chemoinformatics companies by/with large pharmaceutical companies recently. The development in the field of molecular modeling and simulation has played the leading role in the drug design technology in pharmaceutical industry. Starting from Genomics, alignment of genes of interest amongst the species, three dimensional structure prediction from the knowledge of sequence of amino acids, prediction of active sites, searching for lead compounds using database and structure-based design, prediction of binding efficiency prior to the experiment and lead optimization using physico-chemical properties of the compounds are a few to cite. One such case study using in silico attempt towards the designing from known anti-tuberculosis chemicals a set of novel inhibitor and finding the drug target (s) using pathway simulation and analysis [1-3] will be discussed in brief. Recent news has warned the medical community that war against pathogenic bacteria is yet not over, repeated breaking of different drug resistance in different range of pathogen has been observed in the patient especially in developing & underdeveloped countries. Many researchers, probably the next to cancer are experimentally using multi prong attack on the understanding the mechanism and developing new strategy of inhibitors for combating this phenomena, resurging XDR,MDR,PDR. The extensive discussion to define these classes is available in literature [4-7]. Research work engaging with clinician, epidemiologist, biologists, microbiologist etc. in this field is emerging to highlight the complexity of the problem. However, many chemicals has been developed to combat the MDR/XDR Tb yet not been fully successful for a long time. Tuberculii , bacteria have shown to have multiple spontaneous mutations at a predictable rate and independent of different drug administration. Such phenomena are prevalent to many bacterial & more common to viral disease which leads researchers to develop multiple target drug designing. Present discussion will open up the future of drug design using the understanding of disease, its inter relationship within biochemical pathway & effect of protein-protein interaction identified as target for combating persistence stage in bacteria.

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Elucidation of The Binding Modes of Known Small-Molecule Inhibitors at Mycobacterial Atp Synthase Subunits *C* And *E*

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The F_OF_1-adenosine triphosphate (ATP) synthase is a classical anti-tubercular target that has led to Bedaquiline (BDQ), marketed as Sirturo® in 2012 for the treatment of Tuberculosis (TB).A co-crystal structure of BDQbound within the*c*-subunit of mycobacterial ATP synthase was reported in 2015. Meanwhile, the hypothesis made for its binding at another site in the *ε* subunit of ATP synthase needs further exploration. In view of the rapidly emerging drug resistancecases, a molecule targeting multiple sites of ATP synthase is highly desirable to cope up with the drug resistance. In fact, a thorough understanding of the F_OF_1-ATP synthase structure, various binding sites, and structural insights useful in the design of new potent inhibitors are desirable. Therefore, we performed a systematic assessment of the recently resolved structures of subunits c and ε of mycobacterial ATP synthase and explored the inhibitor binding characteristics of few known small-molecule F_OF_1-ATP synthase inhibitors at the BDQ binding site (*i.e.* rotary ring subunit *c*) and the hypothesized druggable subunit ε site.At the subunit *c* site, we observed the importance of E65, Y68, L63, and F69 amino acids of protein that were in direct or water-mediated contacts with the known inhibitors e.g. the hydroxyl and NH groups of BDQ showed hydrogen bonding and salt-bridged interactions that corroborated well with the X-ray based information. Alongside, other inhibitors fitted well at the subunit *c* site and showed a combination of hydrophobic and hydrophilic interactions. On the other hand, at the subunit *ε* site, we delineated the novel potential binding characteristics of these known inhibitors. The structural insights gained in this study may be useful in the design of new small-molecule inhibitors targeting these two sites of the mycobacterial F-type ATP synthase enzyme.

Keywords: ATP synthase, Docking, Tuberculosis, Inhibition, Drug target

Big and Small Data' In Computational Modelling of Toxicological Endpoints

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In the era of traditional toxicology a lot of data has been collected, which are compiled in different data bases (also called ‘small data’). On this basis many Quantitative Structure-Activity Relationship (QSAR) models have been developed with intention to expand the knowledge about toxicity to larger chemical space. On the other side, we have a large depository of ‘big data’, which refers to high throughput screening results and –omics results. It is a particular challenge to compress and integrate the ‘big and small’ data into a single model.

The presentation is oriented to the computational modelling of different toxicological properties considering 'big and small' data. Focus is on representations of 'big data' (genomic and proteomic data) and the application of Counter-propagation Artificial Neural Networks (CPANN). CPANN represent one of the basic algorithms of Artificial Intelligence (AI). In the presentation we introduce their architecture and the training algorithm [1]. An accent is placed on their ability for clustering and classification.

In the talk several studies are introduced. Some studies have been focused to binding affinity to androgene nuclear receptor evaluated with respect to carcinogenic potency data and the CPANN analysis of binding affinities to oestrogen, androgen and glucocorticoid receptors. The clustering of bisphenols with respect to carcinogenic potency database and the developmental toxicity database has been performed with CPANN. Furthermore, several chemometrical studies have been performed on proteomic data using the CPANN, genetic algorithm and the Principal Component Analysis (PCA). The aims are to study the correlation between proteomic data and different in vitro endpoints and to get insight into mechanisms of activity [2]. As example of analysis of genomic data we present the clustering of Zika and Covid virus data regarding the geographical origin of viruses [3].

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Conquering the Neutrophil-A Tale of Novel Neutrophil Serine Protease Inhibitors

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The neutrophils are responsible for our body's innate response against Staphylococcus aureus infections and the main driver of inflammatory processes in human diseases. Recently, our collaborator, Dr. Brian Geisbrecht's lab has discovered family of S. aureus proteins known as extracellular adherence proteins (Eaps). These proteins target immune proteases found exclusively in human neutrophils. The Eaps and their smaller homologues EapH1 and EapH2 are selective inhibitors of neutrophil serine proteases (NSPs), including cathepsin-G (CG) and neutrophil elastase (NE).To better understand the structure basis for inhibition of these NSPs by EapH1 and EapH2, we have carried out NMR chemical shift perturbation (CSP) studies in solution. Our CSP analysis showed that both EapH1 and EapH2 inhibit CG through a similar binding mode, while EapH1 and EapH2 use distinct binding mode to inhibit NE. Our results define a new mechanism of simultaneous inhibition of two serine proteases by a single Eap protein. The understanding how S. aureus blocks neutrophil function may lead us to treating staphylococcalinfections and to develop novel anti-inflammatory inhibitory therapeutics.

Keywords: Neutrophil Serine Protease (NSP), Chemical Shift Perturbation (CSP), Extracellular Adherence Proteins (Eaps), Structure Activity Relationship (SAR).

The Importance of 3D Thinking In Anti-Bacterial Agent Discovery

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3D thinking is very important in drug discovery. 3D thinking helped us in finding Nitreones as drugs. Nitreones are cationic but not very reactive. This is an advantage. Though Nitreones carry two lone pairs of electrons at the central cationic nitrogen, these two lone pairs do not participate in any interactions (including hydrogen bonds). Though nitreones carry two coordination bonds between carbene units and the central nitrogen, these bonds do not participate in any reactions. Hence, nitreones are safe for drug discovery. Metformin, chlorhexidine, famotidine, etc. drugs carry nitreone character. We have been working onthe computational the synthetic aspects of nitreones for the past 15 years. We found a few anti-diabetic, anti-malarial and anti-leishmanial agents carry the niteone character. Recent synthetic and in vitro efforts lead to the discovery of anti-biotic nitreones.

Development of Biased KOR Agonist for managing Chronic Pain

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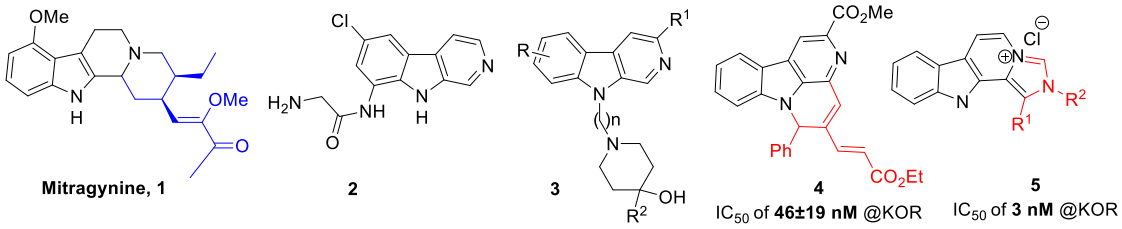
Pain, both acute and chronic, affects millions of people across the globe. Whereas neuropathic pain is usually chronic arising from progressive nerve disease, traumatic nerve injury or infection, non-neuropathic pain (nociceptive pain) is typically due to somatic injury or illness. Opioid analgesics have been long employed as effective method for treating chronic pain but have limitation of serious adverse effects viz. sedation, dizziness, nausea, vomiting, constipation,physical dependence, and respiratory depression.Therefore, many efforts to discovernovel compoundstargeting known pain targets and emerging targets fortreating painare being pursued.[1]

The β-carboline subunit is widely represented in natural sources andbioactive agents displaying activity against different diseases.Mitragynine (**1**), a β-carboline alkaloid which is the major constituent of *M. speciosa* leaves, has opium-like analgesic effect and antitussive properties comparable to codeine but does not produce respiratory depression.[2]Experimental evidence suggests thatmitragynine binds preferably to μ-opioid receptor and κ-opioid receptor (KOR). Another β-carboline derivative 6-chloro-8-(glycinyl)-amino-β-carboline (**2**)is known to display potent inhibitory activity of Nitric oxide implicated as a key factor in the pathogenesis of neuropathic pain.[3]The β-carboline derivative (**3**) is reported to be a potent analgesicsthat acts via selectively inhibiting the GABA uptake.[4] During our work on exploring the potential of fused-β-carbolines for different bioactivities, we have discovered several new β-carbolinederivatives **(4,5)**which displaypotent KOR agonist activity and display better pain relieving activity than duloxetine, the present standard of care. The results pertaining to our study will be presented and discussed.



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Allosteric Changes in Proteins: Earning Extra Miles of Understanding from MD Simulations

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The atoms and molecules in nature are always jiggling and bumping into each other which form the basis of their collective properties. Therefore, the structure-function relationship of molecules in life science is often non-trivial to understand just from the static models of molecular structures. To go beyond, computer simulations offer scopes to witness the atoms in action, mimicking a more realistic behaviour of the molecular structures and tell how exactly they are meaningfully choreographed in order to perform or not to perform a function. But how much it can really help to take the scientific understanding forward? This presentation will address this issue with examples of various molecular systems like α,β-Tubulin [1-5] dimer and TAK1 kinases [6], although with their thermodynamic basis; both of which systems are of tremendous importance in drug design.

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Structure-Based Exploration of Common Food AdditivesToCombatChromosomal Aberration

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Food additives play a crucial role in the preservation, flavor enhancement, and stabilization of commercially available food items. Despite their ubiquitous presence, the potential health implications of these synthetic chemicals have raised concerns. This study delves into the genotoxic effects of food additives, focusing on their interactions with proteins involved in DNA processing, chromatin regulation, and DNA damage repair.n elucidating the mechanisms underlying DNA damage repair, we highlight the intricate pathways orchestrated by cellular machinery to mitigate genomic instability. Furthermore, we delineate the OECD genotoxicity testing guidelines utilized to assess the potential genotoxicity of food additives. Molecular docking emerges as a powerful structure-based simulation for predicting non-covalent interactions between macromolecules and ligands. Leveraging Autodock Vina, molecular docking has been carried out to simulate the interactions of selected common food additives with proteins implicated in chromosomal aberration, DNA processing and repair.

A designer diet for astronauts using the microbiome based approach

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Astronauts travel to space to bring scientific information to benefit humanity under various missions of space agencies such as Indian Space Research Organization, NASA, European Space Agency, etc. Astronauts encounter several stressors during space missions namely microgravity, cosmic radiation, fluid shifts, sleep deprivation and alteration in the circadian rhythm perturbing the quality of sleep. In addition, confined space makes pathogen interaction more probable if a pathobiont gets introduced into spacecraft. Microbiota is the first line ofresistancetovarious disorders and diseases. It directlyinfluences the physiological, biochemical, and immunologicalpathways. 'Gut microbiota' is crucial for healthy gut barrier functions. 'Dysbiosis' refers to perturbation of microbiota which is correlated with several psychologicaland metabolicdisorders. Microbial metabolites are implicated in maintenance of human health. Studies on astronauts in international space missions and on analog terrestrial models have indicated a 'dysbiosis' of the gut microbiota associated with spaceflights. 'Dysbiosis' of the gut microbiome observed in astronauts has been implicated in several disorders including immune dysregulation and a probiotic enriched diet is likely to restore immune homeostasis. We summarized the state of art research on dysbiosis of the gut microbiome of astronauts, but also a diet based on improving the gut microbiome; a viable correction plan to restore astronaut health especially during long term space missions. A characterization of microbial metabolites of the gut to enable administration of astronaut specific probiotic, postbiotic or synbiotic to alleviate space associated dysbiosis has been proposed. It is also proposed that astronauts maintain a balanced nutritious diet throughout life to promote a resilient microbiota that is not perturbed by space missions. Further, a bioregenerative life support system wherein waste re-cycling may be done to produce probiotic space station is proposed.

Keywords: Microbiome, Astronauts, Space agency**,** Diet, Probiotic

Numerical Characterization of Enantiomers and Diastereomers for Quantitative Chiral Structure-activity Relationship (QCSAR) Modeling

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Owing to the homochirality of the building blocks, biological macromolecules like DNA, RNA and proteins are mostly enantioselective towards theirbiological binding partners. In some cases, in the chiral environment a pair of enantiomers may not differ in their relative bio-efficacy very much but sometimes one of the forms may have a superior beneficial or deleterious effect compared to the other. Hence, administration of enantiopure (single enantiomer) drugs is gradually increasing and racemates (enantiomeric mixtures) are getting replaced in the clinical use. As chirality plays an important role in the design of drugs and specialty chemicals, it is essential to include chirality measures in computer assisted drug and molecular design protocols. Most of the chirality measures treat chirality on a binary scale of +1 and -1 and the descriptors thus developed are successful in fulfilling the primary requirement of discriminating the enantiomers and diastereomers. However, these descriptors have limitation in their application because one specific type of descriptors developed for a set of biological molecules may work well for modeling a particular biological activity and will fail when applied to a biological property or efficacy that is mutually uncorrelated to the first one. To make improvementstothis situation, we proposed a suite of new chirality descriptors wherein several of them are mutually uncorrelated. The new family of chirality descriptors called as relative chirality indices (RCIs) were first used [1] to model the mosquito repellent activities of diastereomers of *SS* 220. Subsequently, this approach has been applied to quantitative chiral structure-activity relationship (QCSAR) modeling of opiate σ-receptor and dopamine (DA) D2-receptor affinitiesof seven pairs 3-(3-hydroxyphenyl)piperidines [2]. Recently we extended this approach to QCSAR modeling of CC-chemokine receptor 2 (CCR2) antagonist property of twenty chiral molecules. In this presentation, calculation of the various RCI indices and advantages in using the new chiral descriptors will be discussed.

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FACULTY LECTURES

Applications of Artificial Intelligence in the pharmacy sector

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Artificial intelligence (AI) has become a potent instrument that utilizes personal knowledge and offers quicker fixes for difficult problems. Promising developments in artificial intelligence and machine learning offer a game-changing prospect for drug discovery, formulation, and dosage form testing. Through the application of AI algorithms that examine vast amounts of biological data, such as proteomics and genomics, scientists are able to pinpoint targets linked to disease and anticipate how those targets may interact with possible therapeutic candidates. This makes it possible to approach drug discovery in a more effective and focused manner, which raises the possibility of successful drug approvals. Additionally, by streamlining research and development procedures, AI can help lower development costs. Pharmacokinetics and toxicity of potential drugs can be predicted using machine learning algorithms, which also help with experimental design.This capacity minimizes the need for extensive and expensive animal research by enabling the prioritization and optimization of lead compounds. The broad range of uses of AI in drug discovery, drug delivery dosage form designs, process optimization, testing, and pharmacokinetics/pharmacodynamics (PK/PD) is examined in this thorough overview. For this review I conclude that AI is promising tool for the Pharmacy sector, However, the pharmaceutical industry's ongoing exploration and investment in AI present great opportunities for improving patient care and drug development procedures.

Keywords: Artificial intelligence, Drug Discovery, targeted drug delivery, Proteomics

Proteolysis Pattern of Plant Seed Proteins; An Insight From The Endogenous Peptidome of Germinated And Ungerminated Chickpeas Using LC-MS/MS.

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Proteolysis is a physiological process of protein breakdown into smaller peptides or amino acids with the aid of enzymes. Proteolysis serves many processes such as providing amino acids for new protein synthesis, breakdown of food proteins to provide nutrients, and controlling other physiological and cellular processes. Plant seed proteins, especially legumes are important sources of nutrients, providing an alternative to animal proteins which may have deleterious effects on human health and the environment. However, legumes are less completely digested than dairy or animal muscle proteins. It is known that germination increases protein digestibility of these seeds.

The changes in protein or peptide composition and the pattern of protein hydrolysis which contributes to the increased digestibility upon germination, is not properly understood. The objective of present study was to characterize changes in the peptidome of germinated and ungerminated chickpeas, to gain insights into and changes in active proteolysis preferences, as indicated by changes in motifs at cleavage termini during germination.

We designed a protocol to extract peptides <10kd from 2 different strains of chickpea at 4 different time points of germination. Filtered peptides were prepared for LC-MS/MS and characterised using mass spectrometry, with and without trypsinisation. MS/MS spectra were analyzed using MaxQuant software. Data were visualised using R and Peptigram software.

A clear distinction was seen between the termini of peptides of seeds during the course of germination. Alanine, glutamine and glutamate were preferred at the P1 site (amino acid immediately before the cleavage point) in soaked chickpeas, whereas lysine and arginine dominatedthe P1 position in germinated samples. Principal component analysis indicated that multiple proteases are acting with different substrate preferences. Tiling visualizations of the peptidome for individual proteins indicated the likely activity of exopeptidases. Proteins present in both soaked and germinated seeds are mainly storage proteins and heat shock proteins, whereas proteins specific to germinated samples are enzymes related to the synthesis of new proteins and to the promotion of metabolic activities in growing seedling.

We find that seed proteins are differentially cleaved before and after germination. We identify the preferences of amino acids at different sites of cleavage. These proteolytic preferences have not been previously documented. A better understanding of this natural, large-scale shift in the proteolysis of seed proteins on germination may increase our understanding of how to improve the digestibility of plant proteins.

Keywords
Proteolysis pattern, plant seed proteins, peptidomics

Comperative Analysis of Ligand Binding And Role of Metal Ion In Lectins Using Docking Studies

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Lectins are proteins that can bind carbohydrates. Functions of proteins are related to their three-dimensional (3-D) structures. A major goal of structural biologists is to predict the 3-D structure of a protein which can enhance the understanding of protein-ligand interactions. Molecular modeling techniques can be used to predict the 3-D structures of proteins from their amino acid sequences. Proteins may serve as drug targets for their vital receptor functions. Docking is a key tool to predict the predominant mode of binding of the ligands with the proteins. Structural analysis of the Protein-Ligand complexes can help us to understand their functions in details. Metal ion can stabilize the local conformations of the lectins and make coordination bonds to the acidic residues of the protein and hydroxyl group of the sugar. In this study, formation of complexes of different types of proteins with their specific ligands and metal ions will unfold their mechanism of interactions.

Keywords: 3-D Structure, Molecular modeling, Carbohydrate Recognition Domain (CRD)

YOUNG

RESEARCHERS

ORAL PRESENTATIONS

STRUCTURAL BINDING MODES AND OPTIMIZATIONS OF DUAL FALCIPAIN INHIBITORS USING COMPUTATIONAL APPROACHES

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The emergence *Plasmodium falciparum*resistance to traditional frontline chemotherapies has raised global concerns.Falcipainsdrug target inhibits hemoglobin degradation whichforms free amino acids and are essential for parasite survival. Several potent small-moleculesbeen identified still unable to reach clinical phase due to poor ADMETand off-target specificity against highly homologous human cathepsins.Earlier, we identified two leads **NM12** and **NM15**demonstrating micromolar dual Falcipainsinhibitions. However, their off-target engagement against human cathepsins which are highly conserved remained unexplored. Leveraging computational approach, we studied structural binding modes and selectivity engagementof these leads usingalchemical free energy studies.The leads demonstratedrelatively closer selectivity profiles with both falcipain and cathepsins. Therefore, we further optimized the identified leads to achieve dual falcipain selective binding improvementover cathepsins. The optimized clinical-like candidates exhibited 100 folds higher affinities than the referenceand achieving cell specificitywith falcipains. The molecules were accessed through alchemical studies and newly developed strategies in structural dynamics which endowed in highly potent dual falcipain inhibitors. These optimized leads can be further taken forwet lab studies for developingnew regimen asantimalarial chemotherapy.

Innovative Approaches to Climate-Resilient Healthcare: Harnessing the Power of Pharmacy

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In recent years, the impact of climate change on public health has become increasingly serious, presenting a challenge and deep concern for healthcare systems worldwide. Pharmacy professionals can be among the key stakeholders in addressing this challenge and contribute by playing a pivotal role in combating the challenges enforced by the risk of climate change on human health and the environment. Pharmacy professionals are uniquely positioned to address the health consequences of climate change through a multiprong approach that promotes health and well-being within communities and can contribute to reducing carbon emissions by adopting innovative approaches in the pharmaceutical manufacturing industry and supply chain management. Firstly, they can contribute to the mitigation of climate change by advocating for and implementing environmentally sustainable practices within healthcare and pharmaceutical industry settings. This includes minimizing pharmaceutical waste, reducing carbon emissions from medication production and distribution, and promoting the use of eco-friendly healthcare products. Secondly, pharmacists can actively engage in climate change adaptation efforts by educating patients and communities on the health risks associated with climate change and offering strategies to minimize these risks. This review explores the connection between public health, pharmacy, and climate change. It discusses how pharmacy professionals can play a crucial role in addressing climate-related health issues like heat-related illnesses, air quality concerns, vector-borne diseases, and the sustainable development of the pharmaceutical industry. It emphasizes the importance of collaborative efforts across disciplines to develop sustainable solutions. Pharmacy professionals are highlighted as essential members of interdisciplinary teams working to combat climate change risk and safeguard public health and the environment through innovation, advocacy, and collaboration.

Keywords: Climate change, Public Health, Pharmacy, Pharmaceutical industry, Carbon emission.

DOCKING-BASEDEXPERIMENTAL APPROACH EXAMINING THE EFFECTIVENESS OF NANO-FORMULATIONS AS DIABETES THERAPEUTICS

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Diabetes mellitus is a chronic, metabolic disorder thatneeds to be addressed globally. Diabetes aids in the onset of several associated disorders, including neuropathy, nephropathy, cardiomyopathy, pulmonary arterial disease, etc. Patients develop a reliance on regular medication or insulin dosage, which triggers these related issues. A theoretical validation using computational docking study-based prediction utilizing phyto-based nutraceuticals offers an edge over conventional treatment methods in preventing such situations. The present study explores the potential benefits of plant-based compounds as replacements or alternatives to synthetic pharmaceuticals to improve therapeutic effectiveness while minimizing side effects. Further, to minimize the problems of solubility and dose of phytocompound during internalization, nanotechnology-based drug delivery was explored. Pelargonidin, a phyto-based nutraceutical belonging to the anthocyanidin group known for its therapeutic propertieswhen encapsulated in a biodegradable poly-lactide-co-glycolic-acid (PLGA) polymer, demonstrated increased activity, exceeding that of its non-encapsulated equivalents. Studies using AFM, TEM, and DLS were conducted to determine its physicochemical properties. Therefore, nano-mediated delivery of drugs could improve the solubility, dissolution, retention, and stability of drugs, thereby extending their pharmacological effect.Hence, computational molecular docking studies of drug-protein interactions emerge as a new field aimed at selecting molecules that act to modulate biotargets thereby, establishing the concept of drug delivery with "target-specificity" for combating a variety of diseases including diabetes and its complications.

Keywords: Diabetes, Molecular docking, Nanotechnology, Pelargonidin, PLGA

To Determine the Prevalence of Psychotic illness in Targeted Population

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Background: Bipolar disorder and Schizophrenia are reaction oriented disorders. It particularly originates in childhood which is experienced in later period of life. Kinate receptors are involved in psychotic disorders. **Objective:** The study aims to find out the maximum number of patient suffering from Psychosis in a particular region and different categories of psychotic illness. **Methods**: Inclusion & Exclusion Criteria according to DSM-V & ICD version 2015 (V)- Mental and behavioral disorders were used. **Results**: In case of Bi polar disorder the number of patient found was 280 (Test Sample + Positive Control sample ,Male = 185, Female=95 whereas in Schizophrenia the number of patient found was 160 (Test Sample + Positive Control sample) Male= 99, Female= 61. **Conclusion:** By this study we can conclude that in the prevalence of psychosis disease in the Indian population, "Bipolar disorder and Schizophrenia are the most prominent categories of psychosis in both male and female but the ratio of male is more the female for both the categories.

NANO-PHYTOCOMPOUND COMBATS FOOD-ADDITIVE INDUCED GENOTOXICITY AND MITOCHONDRIAL DYSFUNCTION IN DIABETIC MODEL: AN *IN SILICO* PREDICTED EXPERIMENTAL STUDY

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The study focusses on the therapeutic management of diabetes and associated complicationsinduced by the food additive alloxan(ALX) which isdetrimental to pancreatic β cell functioning. To address the problem, a flavonoid compound Curcumin(CUR) with anti-diabetic, anti-genotoxic, and anti-inflammatory properties, was considered to test its effectiveness in preventing ALX induced diabetic complications based on evidences from molecular docking study. *In silico* study of CUR revealed its interactions with proteins– PARP, p53, bcl-2 and cyt c suggesting a possible function of CUR in modulating cellular cascades.Further, to overcome the problems of targeted and faster drug delivery, drug bioavailability, efficient tissue penetration; nanoencapsulation of CURwas opted as a novel drug-design tool. AFM, DLS, FESEMstudies confirmedphysico-chemical characteristics of newly formed Nanocurcumin(NCUR). As validated by *in silico* docking study, pre-treatment of NCUR in experimental models showed its effective role in restricting genotoxicity and mitochondrial dysfunction by effectively binding with DNA damage repair proteins- PARP and p53 and mitochondrial signaling proteins bcl2 and cyt c respectively.Furthermore, a number of parametric studies have demonstratedNCUR to exert greater efficacy bypreventing tissue damage, delaying incidence of diabetes, DNA damage and chromosomal aberrations.Thus, it can be concluded thatpre-treatment of nano-based phyto- drugs offer promising strategy as therapeutic tool for effective regulation of food-additive induced damages and diabetesvia balancing the expression of proteins involved therein.

KEYWORDS

Diabetes, Alloxan, *In silico* molecular docking, nanocurcumin, genotoxicity, mitochondrial dysfunction

Xenobiotic Induced Obesity Associated Male Reproductive Tract Dysfunction In Drosophila

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Obesity is at the forefront of escalating global public health issues, and WHO's acceleration plan to stop obesity by 2025 for the attainment of SDG 3.4 is in itself a testament that global burden and threat of obesity is a massive public health challenge. Parallel to the conventional factors, recent decades have reported exposure to environmental xenobiotics usually referred to as "obesogens" as an additional factor leading to obesity. Obesogens alter the mechanisms responsible for energy homeostasis and their ability to increase fat deposition results in ensuring their own retention within the exposed organism, given they are lipophilic: a plausible reason as to why obesity serves as an underlying risk factor for so many NCDs', including metabolic syndrome, insulin resistance, reproductive dysfunction, type II diabetes, heart disease, neuropathy, and nephropathy. In the current study, we intend to develop a chemical induced model for obesity and associated male reproductive dysfunction employing *Drosophila melanogaster*. The fruitflies have been exposed to Bis-phenol A (BPA), a widely known endocrine disrupting chemical (EDC), that has recently been classified as a potential obesogen. For modelling obesity the metabolic parameters of the male flies in response to BPA exposure have been assessed by estimating the levels of triglyceride and free glycerol. Later obesity associated male reproductive dysfunction has been assessed by investigating the reproductive parameters of the obese males, that include: reproductive performance of its mate, morphological abnormalities in the male reproductive tissues, sperm fate (production in males and transfer to females), and expression profiling of obesity and reproduction genes that regulate normal metabolic and reproductive function. This study will reveal the cross-talk and triangular relationship between obesogen-obesity and male reproductive dysfunction employing genetically manipulable tools offered by *Drosophila melanogaster and would help us differentiate the pathways perturbed, be it metabolic or reproductive.*

Keywords**:** *Drosophila;* obesogen, BPA, metabolic dysfunction, male reproductive dysfunction

ONLINE / OFFLINE

POSTER

Optimizing Solubility through Co-Crystal Technology: A Rigorous Investigation Into Tablets Loaded With Azelnidipine Co-Crystals

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In the pursuit of enhancing the therapeutic efficacy of Azelnidipine, a widely prescribed antihypertensive agent with limited aqueous solubility, this research delves into the innovative realm of co-crystal technology. The formulation phase incorporates co-crystal strategies designed to optimize the Azelnidipine solubility profile. Three co-formers were employed for co-crystal formulation by wet grinding and solvent evaporation methods. Best Co-crystals were found with co-former saccharine by solvent evaporation methods with the help of different analytical characterization. Azelnidipine-loaded co-crystals using saccharin as a former were compressed in tablet dosage form using the wet granulation method. The evaluation process encompasses a spectrum of pharmaceutical attributes, including dissolution behavior, and stability, ensuring a holistic understanding of the developed dosage form.In-vitro bioequivalent studies form a pivotal component of this investigation, elucidating the comparative pharmacokinetics and bioavailability of the optimized Azelnidipine co-crystal tablet formulation against the conventional dosage form. The findings of this research promise to contribute significantly to the field of drug delivery, offering a comprehensive exploration of co-crystal technology's role in optimizing solubility and bioavailability.

Keywords: Azelnidipine, Co-crystals, Bioequivalence, Solubility Enhancement, Co-former.

Natural Product and Their Derivatives: Promising Caspase-3 Activators Andanticancer Agents

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Cancer is one of the major causes ofglobal morbidity and mortality. The development of various targets found that caspase-3 is an important target whose activation and cleavage may induce apoptosis and ultimately ridfrom cancer cells. Approaching nature for the treatment of cancer is the most demanding for sustainable development. Apart from many synthetic small molecules naturally occurring molecules, have also been reported as caspase-3 activators and inducing apoptosis in the cancer cells. The work presented here will review the published natural products exhibiting caspase-3 activation, or the cleavage to provide some insight into the structural features responsible for caspase-3 activation leading to anticancer activity. This review will help in the development of some novel lead molecules for designing novel molecules of improved cancer therapeutic.The review encompasses the established natural drugs, extracts exhibiting caspase-3 activation and anticancer activity which may be useful for development of lead molecules and optimization of anticancer activity.It may facilitate drug development in a sustainable way.

Keywords: Cancer, Caspase-3, Apoptosis, Natural products

Modeling of he Cyclic Guanidines As 5-Ht$_{5a}$ Receptor Ligands Using Chemometric Tools

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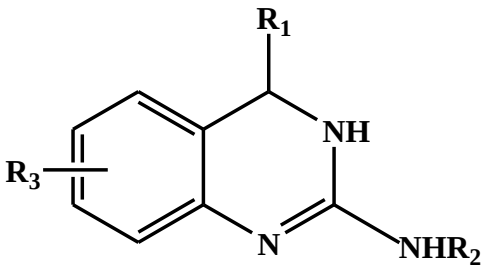

The 5-HT$_{5A}$ receptor binding affinities of the cyclic guanidine derivatives have been quantitatively analyzed in terms of Dragon descriptors. The derived QSAR models have provided rationales to explain the binding affinity of titled compounds. The associations of atomic mass to path length 3 of the Moran autocorrelation (MATS3m), van der Waals volume to path length 3 and 4 of the Moran autocorrelations (MATS3v and MATS4v), polarizability to the highest eigenvalue n.1 of the Burden matrix (BEHp1) and emergence of descriptors Me (mean atomic Sanderson electronegativity scaled on carbon atom) and JGI4 (4th order mean topological charge index) have shown the prevalence of atomic properties and charge content to explain the binding affinity. PLS analysis has also confirmed the dominance of information content of the CP-MLR identified descriptors. The derived models and participating descriptors in them have suggested that the substituents of guanidine moiety have sufficient scope for further modification.

Key words: QSAR, cyclic guanidines, 5-HT$_{5A}$ ligands, binding affinity, PLS, CP-MLR.

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Exploring the Potential of Herbal Nanosponges In Combating The Skin Infections

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Topical drug delivery system faced many problems like poor permeability, skin irritation, allergic reactions.Different types of nanoparticles of plant medicine are gaining a lot of attention currently but they have certain disadvantages like drug loading and toxicity. This research unfolds the potential of nanosponges to conquer these problems. They solubilize poorly water-soluble drug and provide prolonged release. They can load both hydrophilic and hydrophobic drug molecules because of their inner hydrophobic cavities and external hydrophilic branching. Nanosponge are tiny sponges having size of about a virus and can easily penetrate through skin. The outer surface is typically porous, allowing controlled release of drug. Nanosponge drug delivery system has been emerging as one of the most promising fields in drug delivery. Thus, nanosponges loaded herbal formulation not only able to reduce the conventional treatment related to issues but also may serve as future drug delivery carriers for skin care products which improves the patient compliance.

Keywords: Topical drug delivery, nanosponges, increased penetration, improved patient compliance.

Comperative Studies of Some Common Fda Approved Drugs Against Human and Fungal Protein

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The pharmacotherapy that is now available for the management of fungal infections is restricted to medications that fall within the azole, allylamine, echinocandin, etc. categories. Since the fungus strain grows resistant to various treatment classes, we have employed a drug repurposing strategy in this case, investigating currently licensed medications and utilizing computational methods to validate novel therapeutic outcomes.

To explore the new antifungal potential of some FDA approved drugs and comparative studies also validate the results against human protein as well as fungal protein using *insilico* tools.

The selected ligands sdf files obtained from pubchem.ncbi.nlm.nih.gov. & protein of interest data obtained from protein bank .The docking was done by the Prescience *in silico* Solution Suite) version V 2.1.0. The application X-ESS used to PRinS3 and MD – simulations was performed against two proteins humans lanosterol 14-alpha demethylase PDB ID:3LD6 and fungal protein lanosterol 14-alpha-demethylase PDB ID:5V5Z for comparative studies.

In this investigation, the effects of lansoperazole, phenytoin, and atorvastatin were examined. The outcomes were compared with those of commonly used modern medications, such as itraconazole and ketoconazole. By comparing all three drugs against standard medications, the MD simulation was also used to evaluate the stability of the ligands and protein complexes. The average RSMD, COM distance, and interaction energies indicated that all of the chosen drugs formed stable complexes against the proteins that were tested so that for further evaluation proceeds for *invitro* & *invivo* antifungal efficacy studies.

Insilico studies showed that all three drugs showed potential activity against as a potential antifungal drug and is used as an alternative drug against the common fungal strain.

Keywords: Docking, Drug repurposing, Resistance, Minimum inhibitory concentration.

Computer Aided Drug Design For Anti-Tubercular Drug Targeting Electron Transport Chain Pathway

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Tuberculosis (TB) is one of the major leading causes of death worldwide with around 1.4 million death rates as per the World Health Organization (WHO)'s global tuberculosis report 2023.TB causes remarkable mortality and morbidity among people who are immunocompromised or having low immunity e.g., in case of AIDS patients.*Mycobacterium tuberculosis* (Mtb), the causative agent of TB, is highly dependent on the Electron Transport Chain (ETC)pathway for the generation of energy. Mycobacteria opportunistically move to another site for energy generation if anyof its ETC site is inhibited by any drug(Roy et al., 2020). In this study, we aim to design and evaluate novel scaffolds as potential anti-tubercular agents targeting the inhibition of ATP synthase using the docking software "AutoDock Vina". We have considered the X-ray crystal structure of Mtb ATP synthase (PDB-ID: 4V1F) for the docking analysis. We have used Amiloride derivatives, reported as ATP synthase inhibitor, as template for further design of new scaffolds(Hards et al., 2022). We have successfully designed and evaluated new compounds with binding affinity comparable to Amiloride derivative and Bedaquiline, a known drug for TB acting through the same mechanism(Kundu et al., 2016). Further synthesis and biological evaluation of the designed compounds may lead to a potential drug candidate against *Mycobacterium tuberculosis*.

Keywords: Tuberculosis, ATP synthase, Electron Transport Chain, Inhibitor, Scaffold design

Digitalization in Healthcare

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The digital revolution has ushered in a new era of possibilities in healthcare, transforming the way we access, deliver, and manage medical services. This poster explores the multifaceted impact of digitalization on healthcare systems, highlighting key trends, challenges, and opportunities.One significant trend is the adoption of electronic health records (EHRs) and health information systems (HIS), which streamline data management, improve patient information accessibility, and enhance care coordination among providers. Additionally, telemedicine and virtual care platforms have emerged as vital tools, facilitating remote consultations, monitoring, and follow-ups, thus expanding access to healthcare services, especially in underserved areas.Moreover, the integration of artificial intelligence (AI) and machine learning algorithms is revolutionizing diagnostics, treatment planning, and personalized medicine, leading tomore accurate and efficient healthcare delivery. Wearable devices, mobile health apps, and remote monitoring technologies empower patients to actively participate in their health management, promoting preventive care and wellness interventions.However, digitalization in healthcare also presents challenges such as data privacy concerns, interoperability issues, and the digital divide among populations. Addressing these challenges requires collaborative efforts from policymakers, healthcare providers, technology developers, and regulatory bodies to ensure equitable access, data security, and regulatory compliance.In conclusion, digitalization holds immense promise for improving healthcare efficiency, accessibility, and outcomes. By embracing innovative technologies and fostering a culture of digital health literacy, we can unlock the full potential of digitalization to create a more connected, patient-centric healthcare ecosystem.

Natural Drugs to Combat Dengue Fever

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Dengue is a dangerous mosquito-borne, viral infection caused by dengue virus. The female mosquitoes *Aedes* genus is the carrier of these virus . Dengue is a neglectus tropical disease which can kill many lakhs of people around the world because there is no particular small molecules specific chemotherapeutics discovered yet. Major symptoms such as high fever , vomiting, headache, body ache, redness of the skin and head moving happens, after 14 to 21 days of the infection only symptomatic such as acetaminophen, ribavirin, multi vitamins and multi combact dengue. Early diagnosis followed by treatment is urgent . We know that mother gives us birth, feed us and protect from driftful attack of disease. Our universal mother nature has a lots of medicine . The indian traditional medicine such as papaya leafs, giloy, neem, goat milk, curcumin etc. are given to combact to driftful attack of dengue virus.

Development and Assessment of Nanostructured Lipid Carriers Loaded With *Calotropis Gigantea* Extract for the Enhancement of Therapeutic Effect

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The aim of present study was to formulate and evaluate nanostructured lipid carriers (NLC) loaded with *Calotropis gigantean* (giant milkweed) extract prepared by a modified micro-emulsification technique followed by ultrasonication. Nanocarriers have several advantages, such as enhanced solubility and bioavailability of hydrophobic molecules, reduce dose by controlled and sustained release of therapeutic agents, and attenuate drug toxicity. NLC were developed using stearic acid as solid lipid, oleic acid as liquid lipid, Tween 80 as surfactant and Phospolipon 80H as stabilizer. The formulated NLC were characterized for particle size, polydispersibilityindex (PDI), zeta potential, morphology, drug content, entrapment efficiency and in vitro drug release. The optimized NLC formulation exhibited a particle size of 210.46 nm with PDI of 0.256 and Zeta potential of -20.3 mV. Scanning electron microscopy showed smooth spherical morphology. Optimized formulation demonstrated drug content and drug loading capacity of 90.52% and 98.29% respectively. In vitro drug release exhibited sustained release profile, with 75.64% cumulative drug release over 28 hrs following Higuchi release kinetics. Stability studies showed insignificant changes in evaluated parameters over 90 days demonstrating good stability of optimized NLC. The study demonstrates successful development of stable *Calotropisgigantea* loaded NLC with suitable physicochemical properties for topical application.

Keywords: *Calotropis gigantea*, nanostructured lipid carriers, wound healing, micro-emulsification, topical delivery.

Virtual Screening, Admet Profiling, Molecular Docking Approaches To Search For Potent Selective Synthetic Inhibitors Against Kras^{g12d}

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Cancer, a complex and multifaceted group of diseases, is a leading cause of death worldwide. Cancer is characterized by uncontrolled cell growth and the potential to invade surrounding tissues. There are multiple mechanisms reported for cancer pathophysiology. Notably, 25% of cancer cases are due to mutations in KRAS (Kirsten rat sarcoma viral oncogene homolog) protein that result in cancerous cell proliferation and metastasis (Kessler et al., 2019). Recently, the Food and Drug Administration (FDA) has granted fast-track approval to Adagrasib and Sotorasib for use in adult patients with locally progressed or metastatic KRAS^{G12C}-mutated non-small cell lung cancer (NSCLC)(Lanman et al., 2020; Li et al., 2022). In this study, using an *insilico* approach comprised of tool validation, molecular docking, virtual screening and ADMET profiling using the KRAS ^{G12D}crystal structure and commercial database were investigated. We screened7,00,000 compounds from ZINC database. The top-ranked 50 compounds identified from the ZINC database were subjected to ADMET profiling. Molecular docking and ADMET results highlighted a higher affinity of four hit compounds towards KRAS^{G12D} in comparison to the reference inhibitor, BI-2852. Overall, the present research provides strong support for further *in vitro* testing of these newly identified KRAS^{G12D} inhibitors.

Keywords: KRAS, *In silico*, Virtual screening, Molecular docking

Hypertension: A Review

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Objective: The aim of this review is to gather the current information about the various drug therapies and Diagnostic evaluations given to control the disease. **Background:** Hypertension (HTN or HT), also known as high blood pressure (HBP), is a long-term medical condition in which the blood pressure in the arteries is persistently elevated. Blood pressure is defined as the force of blood pushing against the walls of blood vessels. Blood pressure is measured through an apparatus called Sphygmomanometer. Over a billion people around the world have hypertension or high blood pressure. Hypertension is represented by two numbers- The top number is the **systolic blood pressure** which is the arterial pressure when the heart is contracting and the lower number is **diastolic blood pressure** which is the arterial pressure when the heart is relaxing or refilling. The blood pressure which is considered normal is 120/80 mm Hg.

Symptoms : In some patients, the symptoms will develop like Severe headache, Blurred vision, Dizziness, Nausea, Vomiting, Fatigue, Confusion, Chest pain, Shortness of breath.

Diagnostic evaluations-History collection and physical examination (an appropriate measurement of BP), Chest x-ray, ECG, lab tests include blood cell count, blood chemistry (potassium, sodium, creatinine, fasting glucose, total cholesterol and HDL cholesterol)

Management of hypertension: (**A) The life style modification measures mainly include-** Weight reduction, DASH Diet (Dietary approaches to stop hypertension), Dietary sodium reduction, Reduce alcohol, Exercise, Stress management.

B) The Pharmacological therapy includes-Various groups of drugs are used for the treatment of hypertension, collectively these drugs are called as anti-hypertensive drugs, which includes- **Diuretics:** Eg- chlorothiazide, furosemide, **Beta blockers:** Eg- Atenolol, Propranolol ,**Alpha blockers-**Eg: Prazosin ,**Vasodilators:** Eg- Nitroglycerin, Sodium nitroprusside ,**ACE Inhibitors:** Eg- Captopril, Ramipril ,**Calcium channel blockers:** Eg-Amlodipine, Verapamil

Conclusion: High blood pressure causes stroke by causing a break in blood vessels and bleeding in the brain, may lead to impaired vision and blindness, congestive heart failure and can cause the kidneys to fail.

Optimizing Chemotherapy Outcomes: Investigating The Effects Of Fasting And Low-Calorie Diet On Cancer Patients' Health And Treatment Response

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Chemotherapy, a common cancer treatment, often causes distressing side effects that impact patients' health and treatment effectiveness. This study explores whether dietary changes, like fasting or eating fewer calories, can improve chemotherapy outcomes and reduce side effects in cancer patients. Using a randomized controlled trial, a diverse group of cancer patients undergoing chemotherapy will be studied. A comparison will be done between patients fasting and patients on a normal diet. The impact will be validated with the help of various biomarkers and complications associated with Chemotherapy. By closely examining the treatment responses, and how patients feel, the study aims to understand how these diets affect cancer treatment. Previous studies suggest that fasting and low-calorie diets might help chemotherapy work better by making cancer cells more sensitive to treatment while protecting healthy cells. However, it's not clear how these diets work in real-life situations. The study will be carefully planned, ensuring ethical standards and patient safety. The study intends to uncover how fasting and low-calorie diets impact cancer treatment and patient well-being.

The proposed research could change how we approach cancer treatment. If these diets are proven to be beneficial, they could be incorporated and foster cancer treatment and care plans. The outcomes of the study will be crucial in improving treatment outcomes and quality of life for patients. This study also sets the stage for further investigation into the role of nutrition in cancer treatment, potentially leading to more effective therapies in the future.

Keywords :- Low Calorie Diet, Fasting, Patient well-being, Dietary Change

Punarnava Extract: Effective Anticancer Agent

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Cancer is a leading cause of death worldwide and its characterized by uncontrolled growth of cell in the body. Punarnava is an Indian herbal medicine which are commonly found in the region of Uttarakhand its specific name is Boerhavia Diffusa, which consist of anti proliferative and anti estrogenic activity Boerhavia Diffusa having anti cancer properties which has the potential to effectively inhibit the action on Bcl-2 protein and can cure cancer by modifying apoptotic pathways and even Suppressing metastatic genes like TIMP-1, TIMP-2, MMP-2, MMP-9 and VEGF.

Oncolytic Viral Therapy: A Promising Approach in Cancer Treatment

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Oncolytic viral therapy has emerged as a promising and innovative approach in the field of cancer treatment. This therapeutic strategy exploits the selective replication and oncolysis of viruses in tumor cells, while sparing the surrounding healthy tissues. The unique ability of oncolytic viruses to not only directly kill cancer cells but also induce an immune response against tumor antigens has garnered significant attention. In this abstract, we provide an overview of the principles, historical evidances, mechanisms, and potential applications of oncolytic viral therapy. We discuss the different types of oncolytic viruses and their specific mechanisms of action and application of OVs in clinical field. Furthermore, we highlight the challenges and limitations associated with this therapy, such as host immune response and potential side effects. Finally, we discuss future directions to enhance the efficacy and optimize the clinical utility of oncolytic viral therapy, including combination strategies with other treatment modalities. The growing body of evidence supports the potential of oncolytic viral therapy as a valuable addition to the armamentarium of cancer therapy, offering new hope for improved patient outcomes and ultimately, the possibility of eradicating cancer.

Striking A Balance: Unraveling The Relationship Among Corporate Social Responsibility, Sustainability, and Organizational Performance in The Pharmaceutical Industry

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Purpose –

This paper aims to study the inter-relationship among corporate social responsibility (CSR), sustainability and organisational performance in the pharmaceutical sector.

Methodology –

In depth analysis of organizational performance, CSR and sustainability activities of selected 8 pharmaceutical companies was undertaken for a period of consecutive 5 years from 2016 till 2020. This included data collection for the organisational performance variables net income, annual sales and stock market performance parameters (Market capitalization, Price-to-earning ratio and market price per share) for each year. A cumulative score based on the number of activities performed under CSR and sustainability agenda a score was calculated for each selected company for each year. This followed a linear regression analysis to identify whether there is an existence of a relationship among the three entities.

Results –

Both sustainability and CSR positively influence organisational performance in terms of annual sales, and net income (before and after-tax). However, market capitalization and market price per share were negatively influenced by both CSR and sustainability. Another interesting finding showed that price-to-earnings ratios are not influenced by both CSR and sustainability.

Conclusion –

The new insights obtained in the study have further provided real-world evidence to support that both CSR and sustainability improve long-term profits and can be considered investments into the future in the pharmaceutical sector. It advocates investing in activities related to CSR and sustainability initiatives to improve organizational performance which will not only reap profit in the long-term but also do good to the society.

Keywords: Corporate social responsibility, sustainability, pharmaceutical sector, organisational performance, sustainability development goals

Telemedicine and Remote Healthcare

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Particularly in recent years due to the COVID-19 pandemic, **telemedicine and remote healthcare** have experienced tremendous growth and transformation.

An extensive summary of the most recent developments as well as potential future paths in telemedicine and remote healthcare delivery are the goals of this review essay. The study investigated various important aspects such as improved patient engagement, cost-effective delivery models, remote monitoring and management of chronic conditions, availability of emergency and urgent care services, ease of access to specialized consultations and second opinions, integration with electronic health records (EHR), and changes in regulations and reimbursement.

We address the effects of telemedicine on the provision of healthcare, emphasizing its capacity to raise system efficiency, lower healthcare inequities, and improve patient outcomes. We also look at the potential and problems that come with the use of telemedicine, including as technological obstacles, legal issues, privacy issues, and the need for workforce development.

This review clarifies the revolutionary significance of telemedicine and remote healthcare in changing the face of healthcare delivery globally through a thorough analysis of recent literature and case studies. We also note new developments in telemedicine, such as the use of blockchain, wearable technology, and artificial intelligence, and the growth of telemedicine services in niche markets including mental health, geriatrics, and rural healthcare.

Overall, this analysis highlights how important telemedicine and remote healthcare are to enhancing patient-centered care, increasing access to high-quality medical services, and meeting the changing global healthcare needs of society. We highlight the significance of ongoing innovation and cooperation to achieve the full potential of telemedicine in influencing the future of healthcare delivery in our concluding remarks, which include insights into the implications for researchers, policymakers, and stakeholders in the healthcare industry.

Key Words: Remote healthcare, Telemedicine services, Healthcare delivery, EHR, Potential, Revolutionary, Blockchain, Healthcare inequities, technological obstacles.

QSAR Of Repurposed Anti COVID-19 Chemotherapeutics Utilizing Theoretical Structural Descriptors

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By the end of Dec.2019, Novel Corona virus caused COVID-19 erupted from Wuhan China. It was predicted by leaps and bounds and very shortly nCoV attack more than 180 countries around the world. It killed millions of million people, we had been forcefully kept under the lockdown. The economy and livess of the country had been devastated people were crying but there is no small molecule therapy developed till death except few approved vaccines such as covishield, covaxin, coronavac, etc. Natural medicines and few synthetic small molecules such as remdesivir, favipiravir, ribavirin, penciclovir, nitazoxanide, nafamostat, chloroquine(rac), s-chloroquine, r-chloroquine, hydroxychloroquie(rac), r-hydroxychloroquine, s-hydroxychloroquine, umenfenvir, daclatasvir, ivermectin were repurposed to combat covid-19. scientist motivated the chemobioinformatician for the screening of new molecules. That is why it is our objective the present study to develop descriptor based quantitative structure-activity relationship (QSAR) models for the designing of new therapeutics.

Insights Into The Mechanism of Action of Specific Phytoconstituents From The Euphorbiaceae Family, Derived From Docking Analysis.

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Diabetes mellitus (DM) represents a significant metabolic syndrome, affecting approximately 2.8% of the global population with metabolic disorders, a figure projected to escalate to 4.4% by 2030. Among the array of drugs available in the market, including sulfonylureas, biguanides, α-glucosidase inhibitors, thiazolidinediones, and non-sulfonylurea secretagogues, mechanisms such as enhancement of insulin sensitivity, secretion, insulin supplementation, and stimulation of glucose uptake are employed. However, these conventional drugs are often linked to various side effects such as hepatic failure, weight gain, tachycardia, and hypothyroidism. In contrast, herbal remedies offer a promising alternative, characterized by safety, accessibility, fewer side effects, and cost-effectiveness compared to synthetic drugs.Euphorbiaceae, a vast family of dicotyledons boasting 317 genera and 8000 species, yields phytoconstituents like flavonoids, terpenoids, and tannins, which have been utilized in treating ailments ranging from viral infections to skin diseases. While numerous plants within this family have exhibited in vivo antidiabetic properties, the precise mechanism of action of their phytoconstituents remains elusive and warrants further investigation. To address this, docking studies were conducted on the 3D structures of four proteins implicated in type-2 DM, namely 11-β hydroxysteroid dehydrogenase type 1, glutamine: fructose-6-phosphate amidotransferase, protein-tyrosine phosphatase 1B, and mono-ADP-ribosyltransferase sirtuin-6, employing 32 known phytoconstituents from this family. The study's findings, based on docking energies and key amino acid interactions, provide insights into the potential mechanisms of action of these phytoconstituents.

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

Development and Characterization Of Nanosuspension Of An Anti-Cancer Drug To Enhance Therapeutic Efficacy In Gastric Cancer

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Nanosuspensions, distinguished by their reduced particle size and enhanced drug bioavailability, represent a promising avenue to achieve targeted drug delivery in cancer therapeutics. The complicated nature of gastric cancer necessitates innovative drug delivery approaches to enhance therapeutic efficacy. In this study, we present a comprehensive investigation into the development, formulation and characterization of a nanosuspension formulated with capecitabine, an anti-cancer drug, to optimize targeted therapy for gastric cancer. The study focuses on tailoring critical physicochemical parameters, including particle size, zeta potential, drug encapsulation efficiency, and drug release kinetics, to improve drug solubility, absorption, and overall therapeutic efficacy. The capecitabinenanosuspension is designed with the objective of achieving enhanced targeted drug delivery to the gastric tumor site, thereby potentially improving treatment outcomes. The advantages of this approach are discussed, highlighting the potential for increased drug efficacy and the possibility of reducing dosing frequency. The ultimate goal is to bring this novel drug delivery system into clinical settings, providing a promising avenue for more effective and targeted therapy in gastric cancer.

Keywords: Capecitabine, Nanosuspension, Anti-cancer drugs, Gastric Cancer, Targeted Therapy.

Effect of Commonly Used Pesticides On Gut Microbiota

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The widespread use of pesticides in agricultural practices has raised concerns about its potential health effects on humans. This study explores the intricate relationship between pesticide exposure and its detrimental impact on the lungs and gastrointestinal microbiome. When pesticides are sprayed on crops, droplets can be inadvertently ingested or inhaled by individuals without mask working in the fields. Once inhaled, pesticide particles can penetrate to the respiratory tract, gaining access to the lungs. Similarly, ingestion of pesticide through mouth and through contaminated food or water can lead to the entry of these chemicals into the gastrointestinal tract (GIT). Upon entry into the body, pesticides can disrupt the delicate balance of the microbiota residing in the lungs and gut.

Structure-Based Prediction of Biochemical Mechanism of Promising Antimalarial DHFR Inhibitors Utilizing Molecular Docking

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Antimalarial drug discovery remains a crucial endeavor in combating drug-resistant strains of Plasmodium falciparum. In this study, we employed molecular docking techniques to predict the biochemical mechanisms of novel dihydrofolate reductase (DHFR) inhibitors, crucial targets for antimalarial drug development. Through structural analysis and docking simulations, we elucidated the binding interactions between the inhibitors and DHFR enzyme, providing insights into their inhibitory efficacy. Our findings shed light on the molecular basis of antimalarial activity and offer valuable guidance for further optimization of DHFR inhibitors as potential therapeutics against malaria

Pharmacophore Modeling Of Tricyclic Antipsychotics

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Psychiatric problem is a mental disorder characterized by irritation, loss or patience, loss of family touch, abnormal talk and abnormal behavior such as feeling of sadness and depression. Chlorpromazine is widely available as antipsychotic drug used in the treatment of psychotic or schizophrenia. Chlorpromazine contain phenothiazine nucleus having activity against D_2 receptor, but it is not active against 5HT2A receptor therefore it is not used in the treatment of psychosis with depression. Tricyclic antipsychotic dibenzothiazepine, dibenzodiazepine and thienobenzodiazepine conpound shows very good effect against schizophrenia. Pharmacophore modeling of trycyclic antidepressant was established but pharmacophore modeling of trycyclic antipsychotic has not yet been developed. Therefore, distanced based pharmacophore for dibenzodiazepine, dibenzothiazepine, and thienobenzodiazepines derivatives having affinity against dopamine D2 as well as 5HT2A receptors have been generated which may helpful to design further congeneric molecules against depression and psychotic.

IMPACT OF ASHWAGANDHA ON INSOMNIA

Shantanu Tyagi and Sisir Nandi

Insomnia is a sleep disorder that makes it difficult to fall asleep or stay asleep. Symptoms include having trouble falling asleep, stress and anxiety, mental health conditions which are depression, schizophrenia etc. Ashwagandha which is an Indian herbal medicine which is effective to cure the sleeping disorder(insomnia). Its scientific name is withania somnifera, withanolides which is a chemical component of ashwagandha shows effective results to cure insomnia by acting on neurotransmitter (GABA).

Role of Bidens pilosa L. in Health Management

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Biden pilosa is a perennial herb that widely grows all around us. It is commonly known as black-jack, beggar ticks, and farmer's friend's etc. Although it is easily available but it is one of the most neglected medicinal Plants in India having tremendous health benefits. It would not be incorrect to say that it is a kind of plant having various diseases curing potential in single one plant. In many parts of the world it has been traditionally used as a source of food and medicine. In Vietnam, during the Vietnam War, soldiers adopted the herb as a vegetable, which led to it being known as the "soldier vegetable". It is especially important in eastern Africa, where it is known as *michicha*. In traditional Chinese medicine, this plant is considered a medicinal herb, called xianfengcao (Chinese) In traditional Bafumbira medicine, this plant is applied on a fresh wound and is known as inyabalasanya. Extracts from *Bidens pilosa* are used in Southern Africa for malaria. Also there are various scientific and research based studies on *B.pilosa* that shows its Anti-allergy, Anti -hypertensive and smooth muscle relaxant, Anti -cancerogenic, Anti-diabetic, Anti-inflammatory, Anti-microbial, Antioxidant, Antidiabetic, Immunomodulatory Properties , Antitumoral and Antimicrobial etc. All these activities are due to the presence compounds known as polyacetylenes, flavonoids, chalconeokanin, ethyl caffeate, and a hydroxycinnamic acid etc. As *Biden pilosa* has already screened for its potent anti diabetic activity, here in India majority of elderly population are surfing from diabetes, which in long term cause associated disease as well so it call become the choice of drug to treat the diabetes as well associated diseases together by given single drug.

Novel synthesis of 3,5-disubstituted-5*H*-thiazolo[3, 2 -*α*]pyrimidine

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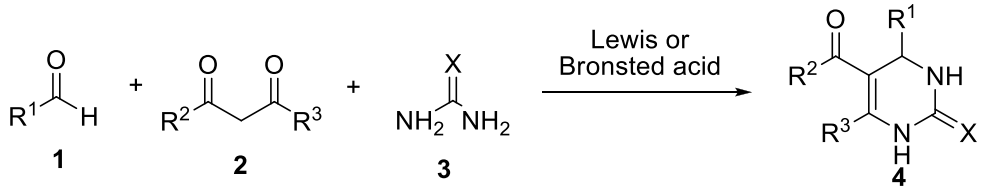
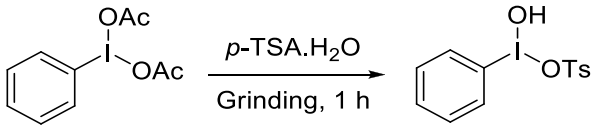
Biginelli reaction are multicomponent (MCR) acid catalyzed cyclocondensation reaction of ethyl acetoacetate **1**, benzaldehyde **2** and urea **3**. The product of this novel one-pot, three component synthesis that precipitated on cooling of the reaction mixture was identified as 3,4-dihydro pyrimidin-2 (*1H*)- one **4** (Scheme 1).

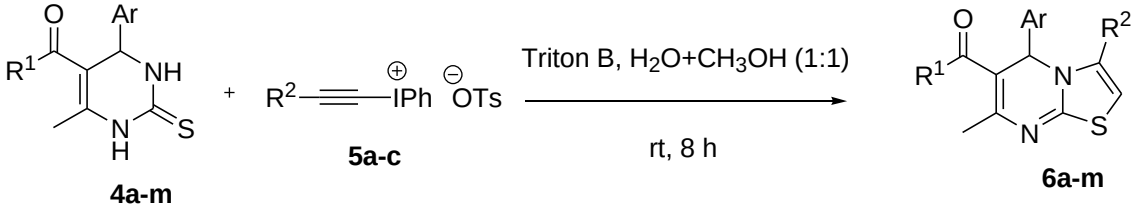


Scheme 1: Synthesis of 3,4-dihydropyrimidin-2-(1*H*)-ones or thiones

A transition metal-free protocol for the synthesis of biologically active thiazolo[3,2-*a*]pyrimidine derivatives has been achieved by the cyclocondensation of 3,4-dihydropyrimidin-2(1*H*)-thiones with alkynyl(aryl)iodonium tosylates. This reaction demonstrates another useful application of alkynyl(aryl)iodonium tosylates as synthon of alkynyl cation.



Herein, we wish to report utilization of the alkynyl(aryl)iodonium salts as another source of building block for the ring annulation of 3,4-dihydropyrimidin-2(1*H*)-thiones to form thiazolo[3,2-*a*]pyrimidine derivatives under transition metal-free conditions. The structural similarity of thioamides and 3,4-dihydropyrimidin-2(1*H*)-thiones led us to envisage that the reaction of the later with doubly electrophilic alkynyl(aryl)iodonium tosylates could lead to form C2-N3 linked thiazolo[3,2-*a*]pyrimidine derivatives and we succeeded (Scheme 14).



Scheme 14: Synthesis of C2-N3 linked thiazolo[3,2-*a*]pyrimidine derivatives

***Keywords*:** Biginelli reaction, thiazolo[3,2-*a*]pyrimidine, alkynyl(aryl)iodonium tosylates, cyclocondensation, hypervalent iodine

Insights Into The Structure And Function Of Caseinolytic Peptidase P From The *Mycobacterium* Genus

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Antibiotics have shown to be of crucial relevance in preventing diseases brought on by dangerous bacteria.However, the irrational antibiotic usage and other confounding factors have led to the emergence of drug-resistant strains.Pathogenic strains of *Mycobacterium* genus have always been a threat to humans. Because of the development of resistance towards the available antibiotics, new antibiotics againstnovel druggable target(s)areurgently needed. One of the prospective targets for the development of novel antibioticsfor tuberculosis is the Caseinolytic peptidase P (ClpP), particularly the pathogenic forms of mycobacteria that infect and wreak havoc on people(1, 2).Understanding the crystal structures of the mycobacterial ClpP can facilitate the design of novel antibioticsagainst it.ClpP is a serine protease that aids in the quality control of proteins in the bacterial cell. It has been reported that changes to the ClpP complex have an impact on the virulence and survival of different bacterial pathogens(3).The hetero-tetradecameric form of ClpP represents the active form.N-blocked dipeptides are necessary for the activation of the ClpP complex leading to proteolysis of misfolded proteins (4). The goal of the current research was to understand the ClpP structure and function, its sequence conservation analysis among mycobacteria, both pathogenic and non-pathogenic, and designing a strategy for the identification of new potential drug that can efficiently kill the drug-resistant mycobacteria.

Keywords: Antibiotics, pathogens, ClpP, drug-resistant, virulence, serine protease

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WEARABLE DEVICES IN HEALTH MONITORING

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Wearable gadgets have evolved quickly, becoming essential components in the field of health monitoring. This abstract investigates the changing landscape of wearable technology, focusing on its transformative impact on personal health and well-being. As these devices grow more common, both consumers and healthcare providers must grasp their different types, benefits, and limitations.

This study classifies wearable devices into three types: fitness trackers, smartwatches, and medical-grade wearables. Each type is examined for its distinct features and functionalities, offering a thorough review of the many tools available for health monitoring. The taxonomy offered explains the rising span of wearable technology, ranging from lifestyle wearables to those built for specialized medical uses.

The advantages of wearable health monitoring are numerous and go beyond basic data collection. Real-time monitoring, tailored information, and the promotion of preventative health practices are some of the primary benefits. This abstract dives into the positive effects of wearables, proving their ability to raise health awareness, promote physical activity, and aid in the early diagnosis and management of health conditions.

Wearable gadgets have significant promise, but they also present issues that must be carefully considered. Concerns about privacy, data security, and the trustworthiness of health data collected by wearables are addressed. Furthermore, difficulties such as user adherence, technological limits, and the possibility of information overload are investigated. Recognizing these limitations is critical for developing a balanced perspective on the use of wearables in health monitoring.

This abstract provides a thorough overview of wearable technologies, including their various varieties, benefits, and problems.

Keywords:- wearable gadgets, fitness tracker, watch, data monitoring

Novel Synthesis of 1-arylnaphtho[1,2-*d*]isoxazole through oxidation of 1-amidoalkyl-2-naphthols using (diacetoxyiodo)benzene

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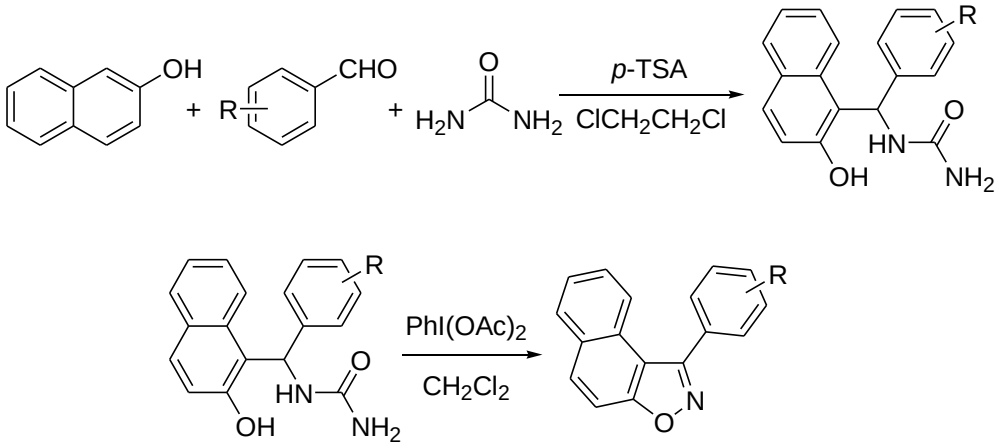
A series of 1-amidoalkyl-2-naphthols were synthesized *via* three component condensation of β-naphthol, aldehyde and urea under acidic conditions. The subsequent reactions of 1-amidoalkyl-2-naphthols with (diacetoxyiodo)benzene resulted in the unusual formation of 1-arylnaphtho[1,2-*d*]isoxazoles. This reaction demonstrates a useful application of (diacetoxyiodo)benzene for the formation of N-O bond.

Keywords: Hypervalent iodine, phenolic oxidation, 1,2-benzisoxazole, 1-amidoalkyl-2-naphthol, 2-hydroxyaryl ketoximes



MicroRNA: The Unseen Regulator of Wound Healing

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Small non-coding RNA molecules called microRNAs (miRNAs) control the expression of genes by attaching to the 3' untranslated regions of their target messenger RNAs (mRNAs) and causing either their destruction or translational suppression. As prospective indicators and therapeutic targets for wound healing, miRNAs are emerging. Here, we give a general summary of the pathogenic process, types, and definition of miRNA. RNA polymerase II or III converts genomic DNA into lengthy primary transcripts (pri-miRNAs), which may contain one or more hairpin forms. The first stage of wound healing, known as hemostasis, tries to control bleeding and avoid infection. At the location of the damage, platelets gather and release several substances, including growth factors, cytokines, and chemokines, which start the inflammatory process. The second stage of wound healing is inflammation, during which immune cells including neutrophils, macrophages, and lymphocytes are drawn to and activated at the site of the injury. The third stage of wound healing, known as proliferation, entails the development of granulation tissue, re-epithelialization, and angiogenesis. Fibroblasts go into the wound area during this phase, when they create collagen and other extracellular matrix elements that give tissues the structural support they need to heal. Several genes, including PTEN, PDCD4, SPRY1, and TIMP3, have a specialized function in the healing of wounds. MicroRNAs including miR-21, miR-146a, miR-155, miR-181a, miR-223, and miR-let-72 are identified as regulators of the inflammatory response in wound healing and have therapeutic potential. TNF-, IL-6, IL-10, TGF-, NF-B, and NLRP3 are examples of inflammatory mediators whose expression is modulated by these miRNAs. This chapter focuses on the obstacles in miRNA therapy, including factors in miRNA target selection and delivery, as well as the miRNAs that may be possibly targeted to improve skin wound healing.

The Influence of the Global Carbon Markets in Mitigating the Risks of Climate Change with Focus on India

Parikshit Narain*, Dr. Kanika Saxena*

Climact **A next generation carbon market platform to shape a climate secure world**

Introduction

Climate change is a real problem facing our generation and the next, with potential impacts threatening our existence. It is a real issue requiring real action on the ground to reduce GHG emissions across the globe. economies globally have recognised the urgency of limiting carbon emissions to fight climate change. This study aims to develop a framework for a digital carbon market to assist in monitoring carbon emissions in India thereby helping in achieving India's commitment to reduce its carbon emission by 45% each year by 2030 and achieve its target of net zero by 2070.

Method

Initially, a literature review was conducted on the role of the carbon market and current greenhouse gas (GHG) emissions in different regions of the world with an emphasis on India. This included studying mobilising green finance towards suppliers by allowing buyers to offset their GHG emissions through verified, high quality and trusted credits. The market structure had following components:

1. Mechanisms to create demand for credits.
2. Supplier and Buyer onboarding
3. Carbon accounting to measure emissions for offsetting
4. Verification to ensure carbon reductions are credible and follow core carbon principles like additionality.
5. Carbon Exchange and trading infrastructure
6. Carbon credit pricing methodology
7. Globally accessible registry
8. Regulatory compliance and reporting
9. Measurement of Co-benefits including SDG compliance for positive impact.

Result

The framework developed is based on the carbon market incentivising emission reductions by assigning a monetary value to carbon emissions, driving investment in cleaner technologies and practices. The framework promotes global cooperation by enabling countries to collaborate on emissions reduction efforts and facilitate the efficient allocation of resources by encouraging emissions reductions where they are most cost-effective.

Conclusion

Fossil fuel consumption, agriculture, land-use change, and cement production are the dominant anthropogenic sources of CO_2in the atmosphere. The digital market space for carbon emissions provided us to not only monitor the carbon emissions but also provide opportunities to reduce the emissions by providing monetary incentives.

Dengue : A Review

Vikas Kori, Shivani Lodha

Faculty of Pharmacy- Veer Madho Singh Bhandari Uttarakhand Technical University, Dehradun

Dengue fever is a mosquito borne viral infection prevalent in tropical and subtropical regions. Dengue is an acute viral illness caused by RNA virus of the family Flaviviridae and spread by Aedes mosquitoes. Presenting features may range from asymptomatic fever to dreaded complication such as hemorrhagic fever and shock. This abstract provide an overview of the disease, encompassing its etiology, transmission, clinical manifestations, and epidemiological significance. Emphasizing the increasing global burden, the abstract discusses prevention measures, challenges in diagnosis, and potential avenues for future research to mitigate the impact of dengue fever on public health.

GIPER High

Impact

Research Credentials

In 2022-23

Academic session

Academic Achievements

The institute generates potential scholars and motivates faculties for incredible work that gives immense outcome in terms of gold medals achieved by the students, awards and recognitions achieved by faculties and the institute.

Students

- Three girl students of GIPER, Kashipur viz. Ms. Vaishali Chauhan, Mrs. Monika Setia and Mrs. Ankita Sharma topped the affiliating university i.e. Veer Madho Singh Bhandari, Uttarakhand Technical University, Dehradun and secured gold medal in B.Pharm, M.Pharm (Pharmaceutics) & M.Pharm (Pharm. Chemistry) respectively in 2022 convocation and Ms. Garima Pandey achieved Gold medal for topped in B Pharm in 2023 convocation.
- Best Poster awards to the GIPER students in national and international conferences.
- M.Pharm student project works have been published in SCI and Scopus indexed journals.
- CADD training to make the students competent.
- Selection of the passed out UG students in Australia & USA for higher study.

Awards conferred to Faculty Members

- Best oral presentation award to Dr. Sisir Nandi, Professor at ITDDD 2018 conference at Punjabi University, Patiala, Punjab.
- Young researcher of the year 2020 award to Mr. Sarfaraz Ahmed, Associate Professor by Shobhit University, Saharanpur, Uttar Pradesh.
- Young achievers award 2021 to Mr. Rajan Kaushik, Associate Professor by Career Point University, Kota, Rajasthan.
- Best researcher of the year 2021 award to Dr. Sisir Nandi, Professor, for outstanding contribution to education skill and research by Centre for Education Growth and Research, New Delhi.
- Principal of the year 2021, to Dr. Deepak Teotia, Director, by Career Point University, Kota, Rajasthan.
- Young teacher award 2022 to Mr. Rajan Kaushik, Associate Professor by Career Point University, Kota, Rajasthan.
- Principal of the year 2022, to Dr. Deepak Teotia, Director, Centre for Education Growth and Research, New Delhi.
- Award for excellence in research 2022, to Mr. Sarfaraz Ahmed, Associate Professor by GTEA Global, New Delhi.

Faculty achievements

Our faculties are generating high-quality work to combat tuberculosis, cancer, Alzheimer's disease, and COVID-19 as proven by the publications in high impact journals like J Med Chem, RSC Adv, Curr Med Chem, Curr Topics Med Chem, Topics Med Chem, Expert Opinion on Therapeutic Patents, SAR QSAR Environ Res, Curr Drug Targets, Curr Pharm Des, etc.

- Dr. Sisir Nandi, Professor & Head (Pharm. Chemistry), published book chapters (Springer Nature, Singapore and Nova Science Publishers, USA, Bentham Science Publishers, UAE)
- Mr. Sarfaraz Ahmed, Associate Professor (Pharm. Chemistry), published a book chapter (Academic Press Elsevier, USA)
- Mr. Rajan Kaushik, Associate Professor (Pharmacognosy), published a book chapter (Apple Academic Press & CRC Press, USA)
- Mr. Rajan Kaushik, Associate Professor (Pharmacognosy), secured Continuing Education Certificates (3.0 AMA/PRA *Category-1 Credits*) from FDA Center for Drug Evaluation and Research, US Food & Drug Administration, USA.

Awards conferred to the institute

Name of Award	Conferring Organization	Year
Brand achievers awards 2015	Brand Achievers	2015
Education excellence awards	Brands Academy	2015
Achievement in business & services awards 2016	Katalyst research	2016
Excellence in Indian education awards 2017	Catalyst Research	2017
Rising star of India- Pharma education	WBR Corp	2017
National Educational Awards	Eminent Research	2018
National Education Excellence Awards	WBR Corp	2019
Best Pharmacy College Uttarakhand	Centre for Education Growth and Research	2019
Educational Leadership Award	Eminent Research	2021
Best Pharmacy College in North India	Centre for Education Growth and Research	2022
Best Pharmacy College in India for Teaching Excellence and Research	Centre for Education Growth and Research	2023
Most Promising Pharmaceutical Education and Research College in Uttarakhand	WBR corp	2023

Books

Anil Kumar Saxena (Ed.), Biophysical and computational tools in drug discovery, Topics in Medicinal Chemistry, Vol 37, 2021

A list of high impact publications of the last three years

Nitin Srivastava, **Anil Kumar Saxena.** Caspase-3 Activators as Anticancer Agents. Curr Protein Pept Sci. 2023.24(10):783-804. Impact Factor 3.0 (Bentham Science; Scopus; Web of Science; Google Scholar)

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Muneer Alam, Zeeshan Fatima and **Sisir Nandi***, Exploring the biochemical mechanisms of fluoroquinolone compounds against tuberculosis utilizing molecular docking and quantitative structure-amino acid relationship, **Letters in Drug Design and Discovery,** 2023**. DOI:** 10.2174/1570180820666230619094409. Impact Factor 1.09.
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