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ACCELERATING Biology 2025

Compute to Transcend

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Book of Abstracts

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DISTINGUISHED GUESTS

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Padma Bhushan Dr. Vijay Bhatkar

Prof. Jayaram N. Chengalur

Prof. Bhushan Patwardhan

Smt. Sunita Verma

Shri. E. Magesh

Shri Sanjay Wandhekar

Dr. Hemant Darbari

Padma Bhushan Dr. Vijay Bhatkar

Chairman, C-DAC Technical Advisory Committee (TAC)

Profile

Honoured with Padma Bhushan, Padma Shri, Maharashtra Bhushan and a string of national awards and Honorary Doctorates, Dr. Vijay Bhatkar is best known as an architect of India's first Supercomputer 'PARAM' and several pioneering contributions to Information Technology in India. He did his Ph.D. from IIT Delhi in 1972 where he was acclaimed as its Distinguished Alumni and went on to become Chairman of its Governing Council. Dr. Vijay Bhatkar has been the Chancellor of Nalanda University, Currently, he is a Member NSM, Chairman, Unnat Bharat Abhiyan, Government of India, Mentor of Vijnana Bharati and guiding India's notable national initiatives in Science and Technology as well as in Arts and Humanities

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Prof. Jayaram N. Chengalur

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Profile

Prof. Jayaram N. Chengalur is a Distinguished Professor and the Director of the National Centre for Radio Astrophysics at the Tata Institute of Fundamental Research, located on the Savitribai Phule Pune University campus in Maharashtra, India. His main research focuses on extragalactic astronomy, particularly the study of nearby dwarf irregular galaxies, neutral hydrogen (HI) absorption in very high redshift galaxies (known as 'damped Lyman alpha' systems), and, more broadly, the evolution of the neutral hydrogen content of the universe.

Prof. Jayaram N. Chengalur obtained his B.Tech. in Electrical Engineering from IIT-Kanpur in 1987. He then moved to Cornell University for his doctoral studies, completing his Ph.D. in 1994. Following this, he worked as a post-doctoral fellow at the Netherlands Institute for Radio Astronomy (ASTRON) in the Netherlands, before joining the National Centre for Radio Astrophysics in 1996. He is a Fellow of the Indian Academy of Sciences, the National Academy of Sciences, India, and the Indian National Science Academy.

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Prof. Bhushan Patwardhan

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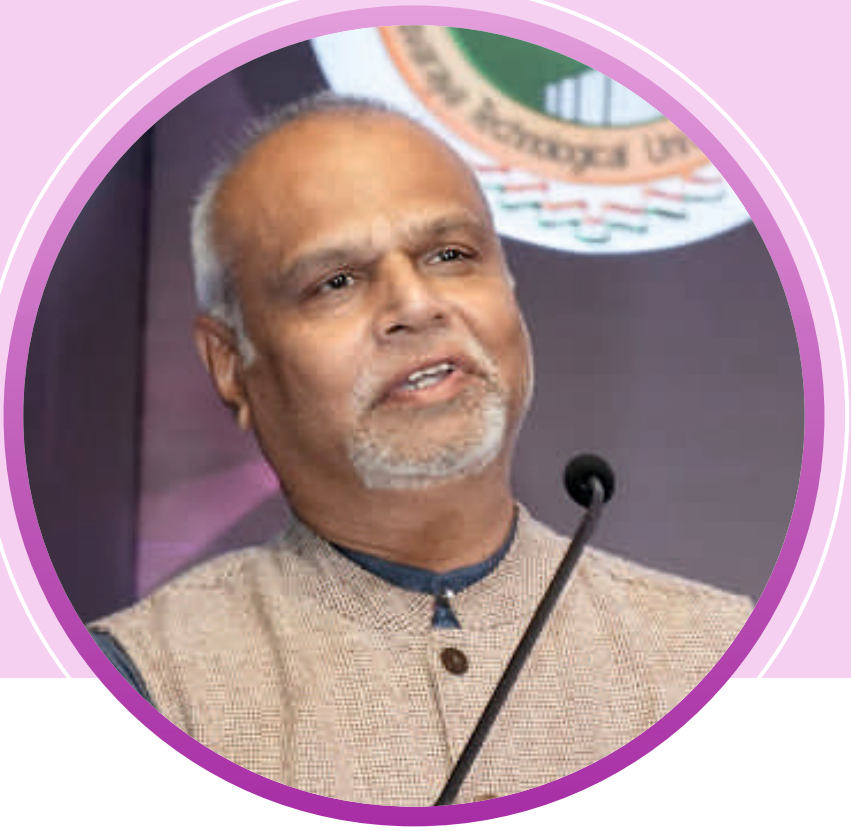

Profile

Prof. Bhushan Patwardhan has over 40 years of experience in higher education, scientific research and institutional governance. He is one of the top cited biomedical scientists who is a Fellow of National Academy of Sciences and National Academy of Medical Sciences India. Until March 2021, he was Vice Chairman, University Grants Commission, and Chairman additional charge Indian Council of Social Science Research, Government of India. Currently, he is Chairman of the Interdisciplinary R&D Taskforce on Covid-19, and member, advisory committee constituted by the Ministry of AYUSH. He is on the taskforce for the proposed WHO Global Center for Traditional Medicine, member National Board of Examination and Lancet Citizen's Commission. Prof. Bhushan is a former Director and currently serving as a Distinguished Professor at the Interdisciplinary School of Health Sciences, and the Center for Complementary and Integrative Health, Savitribai Phule Pune University. He is also an adjunct professor at Western Sydney University, Australia and is a member of the Lancet Citizen's Commission on reimagining India's health system, a senior consultant to the World Health Organization, Geneva. He has made original contributions in evidence-based Ayurveda especially in Ayurvedic biology, ethnopharmacology, natural product drug development and integrative approaches to improve the public health system. His pioneering contributions on novel concepts such as Therapeutic Adjuvants, AyuSoft™, AyuGenomics™,. Reverse Pharmacology, Network Pharmacology are widely recognized. He is recipient of many orations and 14 awards including SASTRA Mahamana Award 2024, Sardar Vallabh Bhai Patel Award 2021, Dr. R.P. Devadas Oration 2020, V K Joag Best Teacher Award 2017 just to mention a few. His World View article on predatory journals published in NATURE has been widely appreciated. It is noteworthy that his 25 articles have been cited more than 100 times. He has received several research grants, has guided 20 PhD students and holds 8 Indian Patents, 2 US Patents with over 9800 citations. Dr Patwardhan's scholarly books 'Integrative Approaches for Health' and 'Innovative Approaches to Drug Discovery' both published by Academic Press Elsevier have received excellent reviews. He has recently published a book titled "Genome to Om" which explores the desired transition from modern science to meta-science, blending ethical, moral, and spiritual insights while recognizing the interconnectedness of all aspects of life.

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Smt. Sunita Verma

Group Coordinator, R&D in Electronics & IT,

Profile

Smt. Sunita Verma is the Group Coordinator for R&D in Electronics &IT at Ministry of Electronics & IT overseeing the entirety of R&D operations including National Supercomputing Mission (NSM). Her pivotal role extends to spearheading the advancement and promotion of Electronics and Information Technology nationwide. This entails crafting policies, evolving R&D proposals, orchestrating their execution, and facilitating their commercialization through collaborative efforts with industrial, academic, and R&D entities. With an extensive tenure spanning over three decades, she possesses a wealth of experience spanning the spectrum of R&D endeavors, from basic research to product development in the areas of Micro-Electronics, Additive Manufacturing, Quantum computing, Circular Economy in E-waste sector, Electronic Materials & Component, Nano Technologies, Medical Electronic and Health Informatics, Electronics Systems Development & Application, etc. Under her supervision, India's first 'Centre of Excellence on E-waste Management', has been established at Hyderabad, India. Wherein, various e-waste recycling process technologies have been developed and transferred to Industries for national benefit. She is heading the National Supercomputing Mission for development and deployment of state-of-the-art Supercomputing facilities in the country. Through her focused and visionary approach, NSM has created a robust ecosystem in the area of High-Performance Computing (HPC) in the country, wherein development of various indigenous HPC sub-components like Server Boards, Interconnect, Software Stack have been undertaken and over 32PF capacity of supercomputers have been deployed across the country. She was instrumental in the development of PARAM SHAVAK machine "Supercomputer in a Box" based on indigenously developed Rudra Server Board. She has played a key role in the development of HPC clusters based on RUDRA Server Board, three of which have been inaugurated by Hon. Prime Minister on 20th Sept 2024.

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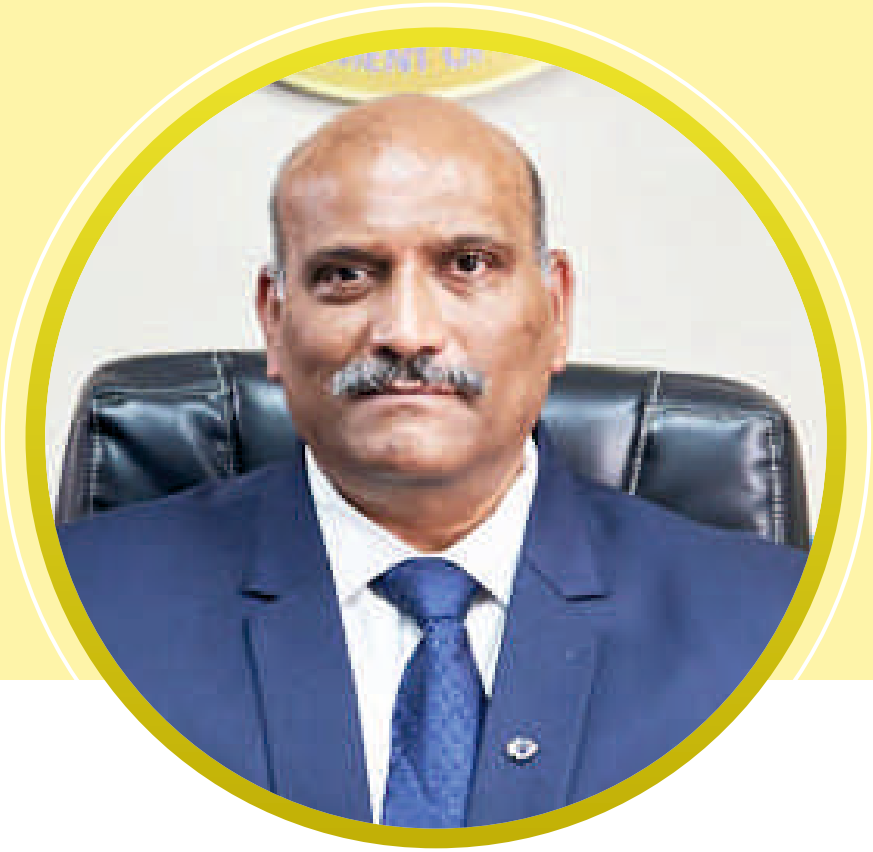
Shri. E. Magesh

Director General, C-DAC



Profile

Shri E. Magesh has been serving in the capacity of Director General, C-DAC since April 2022. He is spearheading the National Mission Programs like the NSM, Microprocessor Development and C-DAC Mission Mode Programs in HPC, AI, Cyber Security, Quantum, Microprocessor and Next Generation Computing. Prior to this Shri Magesh was heading C-DAC Thiruvananthapuram Centre as Executive Director, C-DAC Hyderabad Centre as Director and has also served as Vice President of MNC. Shri Magesh has more than 29 years of diversified experience ranging from Design Engineering, Project Management and delivery of turnkey projects. He has in depth expertise in Electronics and CHIP design, VLSI, Hardware, IP and Complete Product Cycle. He was also responsible for SOC integration, front end to backend, tape-out and silicon validation, interfacing with various functional groups to deliver tested products and managed various ASIC tape-out for customers. Leveraging three decades of his technology expertise, Shri Magesh has significantly contributed towards end-to-end mission planning of national importance, design, integration and analysis. His innovative contributions, particularly the strategies adopted in R&D towards realising 25 Plus ASIC/CHIP, C-DAC's indigenous series 32/64 bit RISCV based of Processor called VEGA, and SOC's called THEJAS under National Microprocessor Development Program, development of 20 Petaflops Supercomputing Facility with indigenous 'RUDRA Server Board', TRINETRA High Speed Interconnect, designing and making our own 'RISC-V based Chip' and 96 core ARM 64bit Processor in 5 nano meter for India first HPC SOC towards Exa-scale computing to 'HPC Storage' to 'HPC-AI Converged Solutions for high level projects of national importance like Safe City including ERSS and Smart Cities, Integrated Cyber Physical Systems, AI based Anomaly Detection for Cyber Security, establishing first of its kind AI Specific National Critical Cloud Infrastructure, HPC-AI Converged Processor has put a good foundation for launch of various indigenous products and solutions making our country self-reliant and in line with the goals of AatmaNirbhar Bharat and Digital India. His visionary approach in conceptualizing ideas in Quantum Technologies is helping to establish a Quantum Computer. This shall enable developing applications to solve grand challenges and societal problems having economic impact leveraging cutting edge scientific research for India's sustainable development.

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Shri Sanjay Wandhekar

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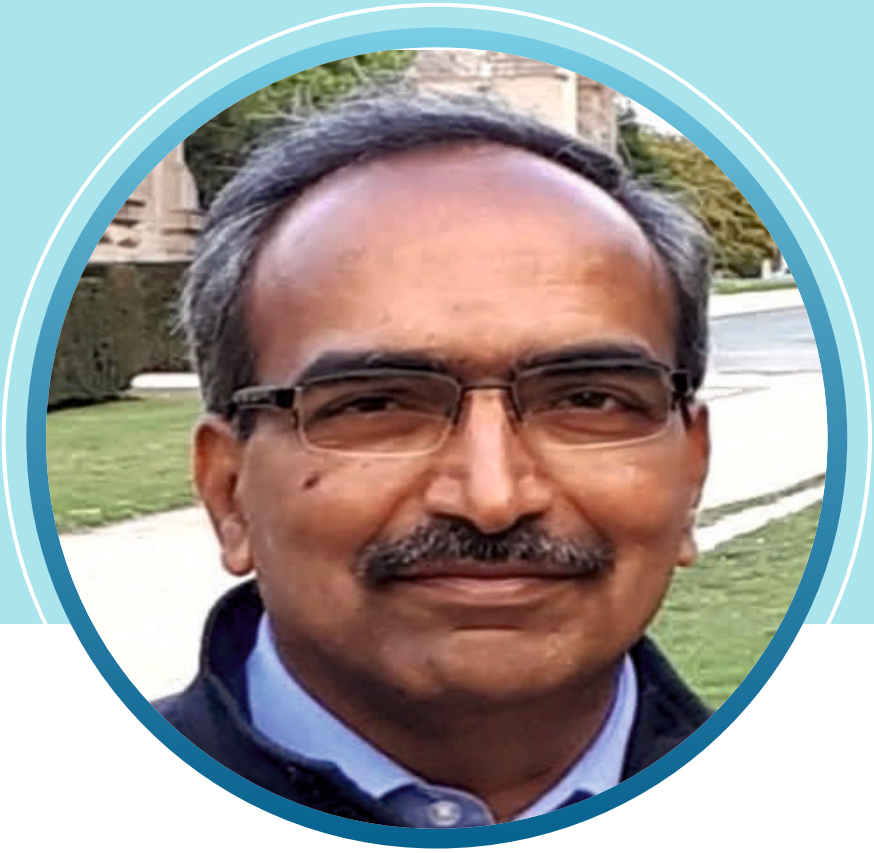

Profile

Shri Sanjay Wandhekar is Centre Head (I/C) of C-DAC, Pune. He is leading the development and establishment of PARAM supercomputing facilities in various institutes across the country under National Supercomputing Mission (NSM). Till date 19 high-end PARAM Supercomputers with cumulative compute power of 30+PF are built and established under NSM. He is alumina of College of Engineering Pune and IIT Kanpur. Sanjay has more than 30 years of management experience in design & development of HPC and IPTV Technologies, and systems. He was a lead member for Development of India's first PARAM series of supercomputers during 90s at C-DAC. He and his team received Dr. A P J Abdul Kalam High Performance Computing Award for Contribution to HPC ecosystem in Year 2019

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Dr. Hemant Darbari

Mission Director, National Supercomputing Mission (NSM)

Profile

Dr. Hemant Darbari is the Mission Director of the National Supercomputing Mission in India. He is an alumnus of IIT- Roorkee and a founding member of the Centre for Development of Advanced Computing (C-DAC). He has an academic background in advanced technological domains and is experienced in areas such as artificial intelligence, machine translation, and high-performance computing. As a Director General, CDAC he was responsible for Building capacity and capability for R&D roadmap in the multi-specialty domains of Multilingual Computing, Software Technologies, Health Informatics, Disaster management, e-Governance and Education & Training. He is the Principal/ Chief Investigator of several projects of national importance like MANTRA (Machine assisted Translation Tool), LILA (Learn Indian Languages through Artificial intelligence), Shrutlekhan (A Hindi Speech to Text System), Shruti-Drishti (Web Browsing through Listening for Visually Impaired), to name a few. Dr. Darbari has received multiple awards and recognitions for his outstanding work in the field of Machine Translation, Speech Technologies, and Hindi language proliferation. He has been honoured with the prestigious "Computerworld Smithsonian Award Medal" and "VASVIK Award" for his contributions to the advancement of Information and Communication Technologies. He has also received the "Award of Excellence in Corporate Leadership" at IIPS-2015 and the "Vishwa Hindi Samman" for his contribution to C-DAC in the field of Hindi Language Computing, Research, and Development.

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SESSION CHAIRS & PANELISTS

Session Chairs & Panelists

- Prof. Ravi P. Mahajan
- Prof. Sunil Sherlekar
- Prof. M. S. Madhusudan
- Dr. Shekhar Mande
- Dr. Sunil Sutar
- Dr. Pragya D. Yadav
- Prof. Andrew Lynn
- Dr. Sangeeta Sawant
- Prof. Arnab Mukherjee
- Dr. Manali Joshi
- Prof. Binay Panda
- Dr. Durba Sengupta
- Dr. Akash Ranjan
- Dr. Rajendra Joshi
- Dr. Uddhavesh Sonavane

Prof. Ravi P. Mahajan

Director of Critical Care Integration and Transformation, Director of Research and Innovation, Apollo Hospitals Group Member of Board of Management, Apollo University, Chittoor Member of Research Advisory Board, AHERF, Hyderabad
Emeritus Professor, University of Nottingham, UK

Profile

Prof. Ravi is a leader in UK Anaesthesia and Intensive Care, more recently as President, Royal College of Anaesthetists. His important international portfolios include Editor in Chief of the British Journal of Anaesthesia (2012-2016); Council member, Royal College of Anaesthetists (RCoA) since 2007; Chairman Safety and Quality Committee, European Society of Anaesthesiology (2012-2016); Chairman, Ethics Committee, Nottingham University (2016-2019); Vice President, Royal College of Anaesthetists (2016-2018) and Medicolegal and Ethics Expert for the court of law in the UK. He has well over 200 Peer-Reviewed International Publications, and has co-authored five textbooks, with his most recent work on Death, Religion and Law. He has successfully established and led a number of international networks and organizations. These include Safe Anaesthesia Liaison Group (Founding Chairman SALG; www.salg.ac.uk); Safety Committee of European Society of Anesthesiology; National Institute of Academic Anaesthesia (Founding Board Member and Chairman NIAA; www.niaa.org.uk); and very recently the Centre for Perioperative Care (CPOC www.cpoc.org.uk) and International Academy of the Colleges of Anaesthesiology.

Professor Ravi's services to the field of medicine, with a long track record of International Leadership in improving patient care through Professional Standards, Quality Improvement, Education and Research, were recognised recently with the award of CBE (Commander of the order of British Empire) in 2022 Queen's New Years Honour List of Great Britain and Commonwealth. In his current positions at Apollo Hospitals Group, he has led the introduction and implementation of comprehensive connected care, a pioneering transformational program for health care delivery in India. He is responsible for bringing in innovative transformational initiatives which require extensive stakeholder engagement alongside interface between technology and medicine, and overseeing international projects from conception to complete roll-out. In addition, he is responsible for overseeing all the aspects related to Research and Innovation.

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Prof. Sunil Sherlekar

Chairman and CEO, SankhyaSutra Labs Ltd., Bengaluru

Profile

Prof. Sunil Sherlekar is the Chairman and CEO of SankhyaSutra Labs Ltd., a company incubated by the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Bangalore and a subsidiary of Reliance Industries Ltd. The company is focused on developing tools for Multiphysics Simulation. He was a member of the Technology Mission for Indian Railways. He serves on the Technology Advisory Committee of the National Supercomputing Mission and on the Executive Committee of Centre for Semiconductor Technologies of IIT Bombay.

Earlier, he was an Adjunct Professor at IIT Bombay and an Adjunct Professor of the Academy of Scientific & Innovative Research (set up by the Council of Scientific & Industrial Research, Govt. of India). He was also an Associate Editor of IEEE Trans on VLSI, on the Steering Committees of Asia & South-Pacific Design Automation Conference and International Conf. on VLSI Design and on the Executive Committee of India Semiconductor Association.

From Sept. 2010 to April 2015, Dr. Sherlekar was the Director of Parallel Computing Research at Intel Labs in Bangalore. Earlier he was the Founder & Head of Research at Tata Computational Research Labs in Pune (2006-2010), the Head of Embedded Systems R&D at Tata Consultancy Services (2002-2006), the CTO at Sasken Communication Technologies (1992-2002) and on the faculty of Computer Science & Engg. at IIT Bombay (1982-1992).

Dr. Sherlekar has a B. Tech. (Elect. Engg.) a M. Tech. (Computer Science & Engg.) and a Ph D. all from IIT Bombay. He is a Fellow of the Indian National Academy of Engineering. He has published several papers in the areas of Electronic Design Automation and VLSI Signal Processing, High-Performance Scientific Computing and a book on VLSI Signal Processing.

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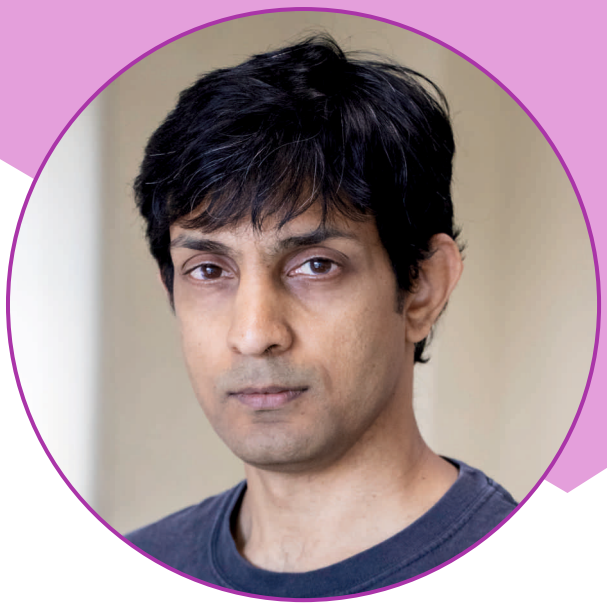
Prof. M. S. Madhusudan

Professor, Indian Institute of Science Education and Research (IISER), Pune



Profile

Prof. Madhusudhan got his PhD in molecular biophysics from the Indian Institute of Science. Following a post-doctoral stint at UCSF he was a PI at BII, Singapore. He is now a professor of Biology and Data science at the Indian Institute of Science Education and Research Pune. His lab works predominantly in the area of computational structural biology.

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Dr. Shekhar Mande

Distinguished Professor, Bioinformatics Centre
Savitribai Phule Pune University, Pune (Former
Secretary, DSIR & Director-General, CSIR)

Profile

Prof. Shekhar Mande, former Director General, CSIR and the Secretary, DSIR, New Delhi is a renowned structural and computational biologist from Pune. He is presently serving as a Distinguished Professor at Savitribai Phule Pune University, Pune. He has served as the Director, National Centre for Cell Science, Pune for more than seven years and is still associated with the institute as the Honorary Distinguished Scientist.

He obtained his Ph.D. from the Indian Institute of Science, Bangalore and went to the University of Groningen, Groningen, The Netherlands for post-doctoral research. He then worked as a Senior Fellow at the University of Washington, Seattle, USA. He began his career as a Scientist C in 1995 at the CSIR-Institute of Microbial Technology, Chandigarh. He worked as a Staff Scientist at the Centre for DNA Fingerprinting and Diagnostics, Hyderabad.

Dr. Mande has received several prestigious awards, including B M Birla Young Scientist Award (1999), Shanti Swarup Bhatnagar Prize for Biological Sciences (2005), BK Bachhawat Memorial Award of the National Academy of Sciences, India, (2017), BC Guha Memorial Award of the Indian National Science Academy, 2017, HK Firodia Award, (2019), and Aryabhatta Medal of the Indian National Science Academy, (2020).

Dr. Mande is a member of several national and international professional bodies. He has been a Wellcome Trust International Senior Research Fellow (2003-08). He is a member of Indian Academy of Sciences, Bangalore (2003), National Academy of Sciences, Allahabad, (2003), and Indian National Science Academy, Delhi, (2010).

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Dr. Sunil Sutar

Industry Process Specialist at Dassault Systèmes

Profile

Dr. Sunil Sutar is a seasoned modeling and simulation expert with over 12 years of extensive industrial experience. He earned his M.Tech. in Design Engineering from IIT Delhi and completed a Ph.D. in Computational Brain Biomechanics from IIT Roorkee.

During his doctoral research, Dr. Sutar focused on blast-induced traumatic injuries, delving into the pathophysiological mechanisms underlying these injuries. His work examined the impact of blast waves on the brain and other body systems, employing advanced modeling and simulation techniques to understand these effects comprehensively. Through his research, he developed effective protection strategies aimed at mitigating the long-term consequences of blast trauma, contributing to advancements in safety and defense mechanisms.

As an Industry Process Specialist at Dassault Systèmes, Dr. Sunil Sutar specializes in the life sciences and healthcare sectors, focusing on the modeling and simulation of virtual human twins, such as the Living Heart Human Model. He develops innovative workflows to evaluate medical device performance, utilizing advanced digital technologies to streamline product development and enhance patient outcomes.

Dr. Sutar's expertise empowers healthcare organizations to visualize and test medical solutions in virtual environments, improving the efficiency and accuracy of medical device design and testing. By integrating cutting-edge simulation techniques, he plays a pivotal role in advancing personalized healthcare and optimizing medical technologies for better patient care.

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Dr. Pragya D. Yadav

Director in Charge, National Institute of One Health, Nagpur Scientist F & Group Leader, Maximum Containment Laboratory, ICMR-NIV, Pune

Profile

Dr. Pragya Yadav is currently working as Director-in-charge, National Institute of One Health, Nagpur and Scientist 'F' and leading Asia's first Biosafety Level-4 laboratory at Indian Council of Medical Research-National Institute of Virology (ICMR-NIV), Pune, India. With her extensive experience in the field of virology, she has contributed significantly to the understanding of emerging viral infections in India. She has obtained PhD in Virology from the Savitribai Phule Pune University, Pune in 2004 and joined as a Scientist in ICMR-NIV, Pune. Since then, actively involved in the surveillance and research of emerging viral infections. She had make significant contributions in the field of virology and biocontainment science, human and animal Virology, health sciences, epidemiology, biomedical sciences, molecular biology, public health, research & development, biocontainment science, translational research, and preclinical vaccine studies in animal model with the special focus on highly infectious viral pathogens. The two decades of experience of working on highly pathogenic Risk group-3 & 4 viruses have added advantage to the public health system in timely identification and containing the outbreaks in the country. Dr. Pragya Yadav is a distinguished scientist with 330 publications, over 10,335 citations, and an impressive H-index of 47. She is a Guest Editor for leading journals such as Virology and Frontiers in Virology. Dr. Yadav is a Fellow of prestigious academies, including the National Academy of Medical Sciences (NAMS), National Academy of Agricultural Sciences (NAAS), and the Indian Virological Society (IVS). Her expertise is internationally recognized, and she serves as an expert for organizations such as the World Health Organization (WHO), Coalition for Epidemic Preparedness Innovations (CEPI), Indian Council of Medical Research (ICMR), and Department of Biotechnology (DBT). Dr. Yadav has also been recognized as one of the top 2% scientists globally, as listed by Stanford University and Elsevier.

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Prof. Andrew Lynn

Professor, School of Computational and Integrative Sciences(formerly known as School of Information Technology) Jawaharlal Nehru University, New Delhi

Profile

Prof. Andrew Lynn is currently a Professor at the School of Computational and Integrative Sciences at Jawaharlal Nehru University, where he has been a Dean, and Coordinator of the Center of Excellence in Computational Biology and Bioinformatics, as well as Director of Communication and Information Services. He has served on the Board of Studies in the area of Bioinformatics. His areas of research are predominantly in Computational Biology and Biomedical Data Science: where he works on development and deployment of computational methods applied to biological sequence, structure and systems analysis. Specific contributions include the use of Hidden Markov Models for functional identification of proteins, which has been pioneered through the development of HMM-ModE. Methods that improve small molecule docking scores, cheminformatics using data-mining methods, simulations of macromolecular systems, analysis of high-throughput data from biological experiments, and application of data-mining in healthcare is the current focus of the lab in this area. Additional interests are in Cyberinfrastructure, where he established the university High-Performance Computer Facility and managed the university IT infrastructure, including with the Open Source Drug Discovery (OSDD): within which he managed responsibilities associated with the technical and grid infrastructure along with project management through the Technical, Science and Budget committees. With this project, he provisioned methods for target, as well as ligand, based lead identification and pioneered the use of crowdsourcing for annotation, development and deployment of applications.

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Dr. Sangeeta Sawant

Director, Bioinformatics Center,
SPPU, Pune

Profile

Dr. Sangeeta Sawant is Director of Bioinformatics Centre, Savitribai Phule Pune University and has an experience of teaching and research in Bioinformatics for more than 25 years. She has contributed to development of bioinformatics resources as well as application of computational methods to biological data for predictive analysis. Her research areas of interest include Structural Bioinformatics, conformational properties of oligopeptides and structure-function relationship studies of key proteins involved in various biological processes and diseases such as Leishmaniasis, diabetes and cancer. The research contributions by Dr. Sawant include development of an algorithm for prediction of conformational states, development of MD simulation-based approach for prediction of oligopeptide structures, characterization of various drug and vaccine targets for leukemia, Leishmaniasis and Japanese encephalitis using molecular modeling and simulation based approaches. She has research projects and collaborations with fellow faculty members from SP Pune University, national R&D laboratories and University of Southeast Norway (formerly Telemark University College). She has to her credit several research publications in international peer-review ed journals and two book chapters. She holds a joint multi-state patent for development of chimeric peptide vaccine for Japanese encephalitis, along with colleagues from Bioinformatics Centre and National Institute of Virology, Pune. She has been involved in teaching various courses such as Biological Databases, Biomolecular Sequence Analysis, Structural Biology and Bioinformatics, Genomics, and Molecular Modeling & Simulations. In addition to teaching in the M. Sc. Bioinformatics program, she has also contributed to the teaching of Bioinformatics courses to the students of M. Sc. Biotechnology, Microbiology, MBA Biotechnology etc. She has served as a member of Board of Studies of Bioinformatics and made significant contributions to development of the syllabi of M.Sc. Bioinformatics.

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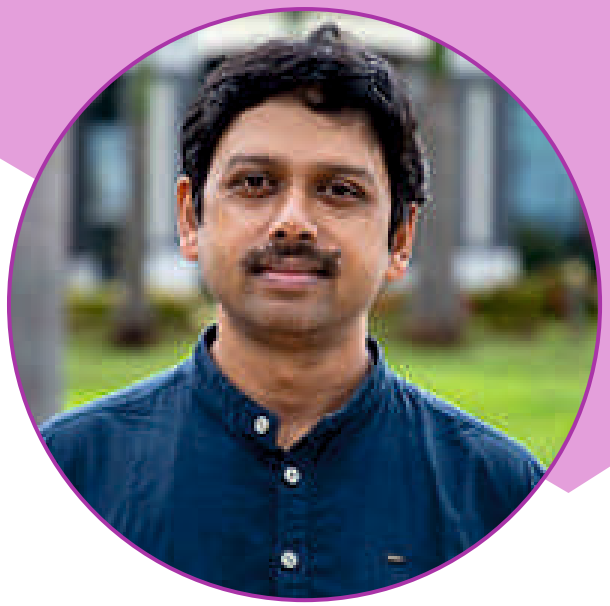
Prof. Arnab Mukherjee

Professor, Indian Institute of Science Education and Research (IISER), Pune



Profile

Prof. Arnab Mukherjee did his B. Sc from Jadavpur university, Kolkata in 1998. He then joined Indian Institute of Science, Bangalore as an integrated PhD student in chemical sciences. He completed his Ph. D. from S. S. C. U. department of IISc Bangalore in 2005 under the supervision of Professor Biman Bagchi. Dr. Mukherjee then went for his postdoctoral research in ENS, Paris, France from 2005 to 2007 and then to University of Colorado, Boulder from 2007 to 2009. He then joined IISER Pune as an assistant professor in November, 2009. He became associate professor in 2015 and full professor in 2021.

Dr. Mukherjee works on the computational biophysics area such as drug-DNA intercalation, DNA structural change, single water entropy, protein folding and protein-DNA binding, dynamical recrossing and internal friction in proteins, etc. He also collaborates with experimental colleagues in various projects such as synthetic ion channels, spectroscopic investigation of molecular recognition, etc. Recently, he ventured into structure-based drug design using both classical interaction and reinforcement learning approaches.

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Dr. Manali Joshi

Assistant Professor, Bioinformatics Centre,
SPPU, Pune

Profile

Dr. Manali Joshi is a computational structural biologist, currently working as an Assistant Professor at the Bioinformatics Centre at S. P. Pune University. Dr. Joshi has a Master's degree in Biotechnology from IIT Bombay and PhD in Biochemistry from University of Houston, Texas. Dr. Joshi is interested in using and developing computational tools to understand the Structure - Function - Inhibition paradigm of several interesting proteins including GPCRs and Kinases. Recently her group has
also started work related to Ayurveda and Plant Biology. Dr. Joshi works in close collaboration with several experimentalists across the world.

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Prof. Binay Panda

Professor, School of Biotechnology &
Special Centre for Systems Medicine
(Concurrent Appointment), Jawaharlal
Nehru University, New Delhi

Profile

Prof. Binay Panda is a Professor at the Jawaharlal Nehru University, New Delhi. His lab focuses on Disease and Computational Genomics and Integrated Biological Data Analysis. He received his Doctorate Degree from the University of Oxford, UK, and Post-Doctoral training at the Scripps Research Institute, La Jolla, California, USA, with a Fellowship from the American Cancer Society. Binay was a Visiting Researcher of Genome Science at the University of Tokyo, Japan, and a visiting Professor at the Technical University, Denmark

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Dr. Durba Sengupta

Principle Scientist and Associate Professor (AcSIR)
National Chemical Laboratory, Pune

Profile

Dr. Durba Sengupta is currently a scientist at the National Chemical Laboratory, Pune and an Associate Professor at AcSIR, Ghaziabad. She has been awarded a doctoral degree from the University of Heidelberg, Germany. Subsequently, she joined the University of Groningen, Netherlands as a postdoctoral researcher. The main interest of her research group is computational biology, in particular multi-scale simulations. They have been able to identify the molecular mechanisms underlying several processes such as membrane protein dynamics, and protein-lipid interactions, and work in close collaboration with experimentalists. She has published several articles in internationally reputed journals, and has been invited to multiple international conferences in biophysics and computational biology. Dr. Sengupta is an editor of J. Membr. Biol. (Springer Nature Press) and an editorial board member of Proc. India Nat. Sci. Ac. and has guest edited special issues for these two journals.

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Dr. Akash Ranjan

Computational & Functional Genomics
Group, CDFD, Hyderabad

Profile

Dr. Akash Ranjan is a renowned computational biologist with a passion for unraveling the mysteries of human disease. His current research focuses on discovering novel functions of biomolecules and understanding their role in molecular mechanisms associated with disease biology.

Dr. Ranjan has published numerous high-impact research papers in leading scientific journals. His work has led to the development of cutting-edge computational tools for analyzing biological data. He has mentored and trained numerous Master and PhD students. He has served as a key contributor to several national and international research projects.

Dr. Ranjan holds a Ph.D. in Computational Biology and Biotechnology of Baculovirus-based expression vector system from the National Institute of Immunology, New Delhi, and a Master's degree in Biotechnology and a B.Sc. (Hons.) in Human Biology from the All India Institute of Medical Sciences (AIIMS), New Delhi. Dr. Ranjan's research interests include Computational structural biology, Functional genomics, Disease modeling, and Systems biology.

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Dr. Rajendra Joshi

Scientist G and HOD,HPC: Medical and Bioinformatics Applications,Centre for Development of Advanced Computing (C-DAC), Pune

Profile

Dr. Rajendra Joshi holds a Master's degree in Biochemistry from the University of Pune, and a Doctorate in Biochemistry from National Chemical Laboratory, University of Pune. He has also served as faculty member at the Bioinformatics Centre, University of Pune. He brings with him industrial experience from his previous work on the development of vaccines. His association with biotechnology and bioinformatics spans more than 25 years. He is primarily responsible for building a strong bioinformatics group at C-DAC and is currently a Scientist G and the Head of the Department at C-DAC, Pune. He has been instrumental in setting up the Bioinformatics Resources and Applications Facility (BRAF) which serves as a nodal point for all the life-sciences researchers who require high speed computing. BRAF has created collaborations within India and across the globe. Dr. Joshi has been leading a number of large projects, including those involving development of advanced workflows and software for automated genome analysis. His main research interests include, molecular dynamics simulations of nucleic acids and proteins, genome sequence analysis, metabolic pathways and development of problem-solving environments. He has been conferred the prestigious VASVIK award for year 2022 for his contribution in use of HPC for biological research. He has more than hundred publications, articles and invited talks to his credit.

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Dr. Uddhavesh Sonavane

Scientist F, HPC: Medical and Bioinformatics Applications, Centre for Development of Advanced Computing (C-DAC), Pune

Profile

Dr. Uddhavesh Sonavane completed his Bachelors and Masters (Physics) degree from University of Pune. He received his Ph.D in Physics in 2002 from National Chemical Laboratory, Pune, India. He has more than 20 years of experience in the area of molecular modeling/ simulations of cancer proteins, quantum chemistry of RNA modifications, antisense molecules. He is currently working as Scientist F at C-DAC bioinformatics group at Pune. He has authored more than 70 publications. He has visited different countries like US, Japan to participate in the conferences and UK as a part of scientific exchange.

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VALEDICTORY SESSION

Dr. Deepak Ranade

Director & CEO, Spinexpertz, Consultant Neurosurgeon,YCM Hospital and Institute of Post Graduation
Honorary Faculty, MIT-WPU School of Consciousness Studies

Profile

Dr. Deepak Ranade was a Professor of Neurosurgery in a University Hospital in Pune. He set up the Department in 2001 and since then the Department has become one of the most reputed with state-of-the-art technology and equipment. It is a recognized center for Neurosurgical Training. He has recently started his own centre of Spine Surgery that offers comprehensive spine surgical facilities.
Dr. Ranade has published more than 30 papers in International Journals. He has one of the largest series in the country for anterior approaches to the dorsolumbar spine.
He is an avid trekker having completed more than 14 high altitude treks in the Himalayas. He is also a writer of repute and has contributed more than 120 articles in the Speaking Tree column of the Times of India, the national newspaper in the fields of Consciousness, Quantum Physics, Spirituality. He is also a self-taught Saxophonist, and guitarist and has given more than a dozen public performances.
Presently, he is pursuing a PhD in 'Role of the Default Mode Network in genesis of Consciousness and the Sense of Self.'

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SPEAKER PROFILES & ABSTRACTS

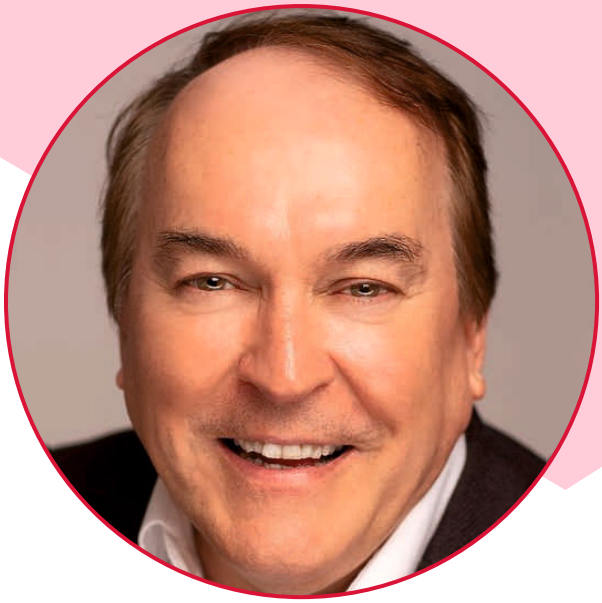
Session: Digital Twins in Biology and Medicine

Prof. Peter Coveney

Dr. Eric Stahlberg

Prof. Peter Coveney

Director, Centre for Computational Science (CCS) & Professor of Physical Chemistry, University College London



Profile

Peter Coveney is a Professor of Physical Chemistry, Honorary Professor of Computer Science, and Director of the Centre for Computational Science (CCS) and Associate Director of the Advanced Research Computing Centre at University College London (UCL). He is also Professor of Applied High Performance Computing at the University of Amsterdam (UvA) and Professor Adjunct at the Yale School of Medicine, Yale University. He is a Fellow of the Royal Academy of Engineering and Member of Academia Europaea. Dr Coveney has made outstanding contributions across a wide range of scientific and engineering fields, including physics, chemistry, chemical engineering, materials, computer science, high performance computing and biomedicine, much of it harnessing the power of supercomputing to conduct original research at unprecedented space and time scales. He has shown influential leadership across these fields, manifested through running multiple initiatives and multi-partner interdisciplinary grants, in the UK, Europe and the US.

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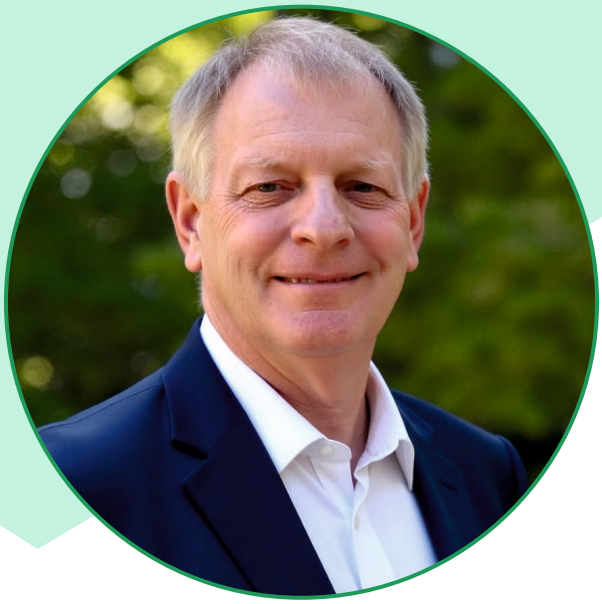
Digital You: The Virtual Future of Medicine

Abstract

The virtual human concept is a compelling one, offering an/in silico/ environment — now known as a digital twin — within which truly personalised medicine can be implemented, taking into account the specific features of every one of us as an individual, from our personal genome to the anatomy of our connected organ systems, and beyond into human populations and clinical trials. Such virtual humans will not only support medical and clinical treatment and decision making, they will also reduce the need for animal testing and serve as personal avatars which will assist every one of us in making healthcare and lifestyle choices. The theory, modelling, software and computational challenges associated with the virtual human are immense and will require many years of intensive research effort to bring to fruition. However, the modern principles of modular assembly of tried and tested components will take advantage of the considerable progress already being made in many aspects of the overall virtual human. Indeed, building virtual humans presents a multiscale challenge, as we must integrate data and models at every level ranging between molecular, subcellular, cells, tissues and organs (and even beyond the single human to population health to address epidemiological issues). My talk will exchange recent breakthroughs in HPC and make comparison with other ambitious digital twin projects underway today and outline several biomedical issues which are being addressed today, based on various components of the future virtual human. These examples illustrate how future patient-specific medical treatments will draw increasingly on the massive power of modern IT systems, including big data, artificial intelligence and supercomputing.



Dr. Eric Stahlberg

Executive Administrative Director
Institute for Data Science in Oncology, UT MD
Anderson Cancer Center, Houston TX

Profile

Dr. Eric Stahlberg is the Executive Administrative Director of Institute of Data Science in Oncology at UT MD Anderson Cancer Centre, Houston TX. He has directed cancer data science initiatives at the Frederick National Laboratory. He has been instrumental in establishing the Frederick National Laboratory's 2014 HPC initiative and in assembling collaborative teams across multiple, complex organizations to advance predictive oncology.

Stahlberg has played a leadership role in many key partnerships, including forming the groundbreaking 2016 collaboration between the US National Cancer Institute and the US Department of Energy where the agencies are accelerating progress in precision oncology and advanced computing applications. He also has been instrumental in forming the Accelerating Therapeutics for Opportunities in Medicine (ATOM) collaboration in 2017 where he continues to fill leadership roles shaping the future for collaborative drug discovery. He has led FNL program efforts establishing foundations for digital twin applications in cancer, and now advancing personalized medicine for all individuals through virtual human models and digital twin approaches. He co-organizes the annual Computational Approaches for Cancer at SC and HPC Applications of Precision Medicine workshops at ISC as well as cross-government workshops with the US FDA. Most recently, he spearheaded the first Virtual Human Global Summit in October 2023. Dr. Stahlberg has undergraduate degrees in chemistry, computer science and mathematics and a PhD in theoretical chemistry from the Ohio State University. He has been at the leading-edge of HPC applications throughout his career, earning honorable mention in the Intel Grand Challenge competition while as a post-doc at Argonne National Laboratory, developing cross-platform scalable parallel computing applications while at Cray Research Inc., pioneering quantum chemistry applications for the first versions of OpenMP and advancing interoperability standards for FPGAs. He has been recognized as one of the FCW top 100, received the President's award from Frederick National Laboratory, and has received the distinguished alumni award from his alma mater, Wartburg College.

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Cancer, Data Science, and Prediction in Medicine: Perspectives for the Future

Abstract

The convergence of computing, predictive analytics and growing sources of data has created a rapidly expanding frontier for the development of new approaches to integrate biological, medical and personal insights to advance research, improve reliability, and better inform patient care. The emergence of biomedical digital twins is revealing important new insights and leading to new exciting questions as these approaches progress from vision to practice, particularly in the challenging area of cancer. The presentation will share important lessons learned and explore forward looking perspectives in areas including collaboration, data, and trust as the digital transformation in medicine accelerates towards a future of integrated personalized and predictive health.

Session: Transcending Technologies and Enablers

Dr. Rossen Apostolov

Prof. dr. A.M.J.J. (Alexandre) Bonvin

Ms. Jaya Panvalkar

Shri Sanjay Wandhekar

Dr. Rossen Apostolov

Director at BioExcel CoE, Group Lead
HPC Software R&D at PDC Centre for High Performance Computing, KTH Royal Institute of Technology, Sweden

Profile

Dr. Rossen Apostolov is Director of BioExcel Centre of Excellence (www.bioexcel.eu) and Group Lead of HPC Software Research & Development team at PDC Centre for High Performance Computing at the KTH Royal Institute of Technology. He is Chairman of the European HPC CoE Council and leader of the European teams in GANANA, the EU-India Partnership for HPC in Scientific Computing. His interests are in the development and application of modern HPC technologies for computational Life Science research, policy development and international collaborations in the field.

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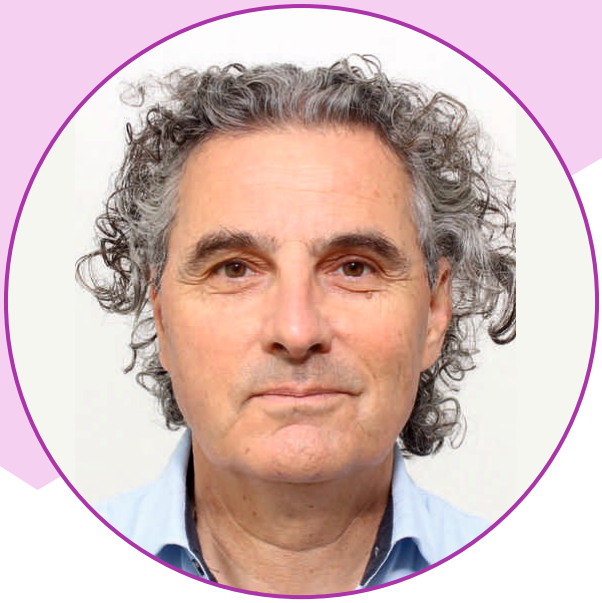
Advanced Methods and Applications for Extreme-Scale Biomolecular Simulations & EU-India collaboration efforts

Abstract

Modern supercomputing systems allow us to run simulations of biomolecular systems of ever-growing size and complexity. Achieving fast and accurate results of the simulations requires advanced computational techniques capable of handling extreme-scale data and processing demands while efficiently using diverse ecosystem of hardware architectures. This presentation explores state-of-the-art methods with emphasise on scalable modeling and parallelization algorithms. We highlight recent innovations in GPU-accelerated processing, extreme-scale HPC and Cloud simulations and usability automations with key applications in structural biology and biophysics.
The presented work is part of the basis of GANANA, an upcoming EU-India partnership on scientific HPC. By combining resources and expertise from both regions, GANANA aims to facilitate shared access to cutting-edge hardware, port and deploy key software, develop jointly optimized algorithms, adopt best practices for applying HPC to select key scientific problems and strenghten the links between research groups. The partnership will be a basis for establishing a long-term collaborative framework for EU-India activities.



Prof. dr. A.M.J.J. (Alexandre) Bonvin

Professor of Computational Structural Biology
Faculty of Science, Utrecht University, Netherlands

Profile

Dr. Alexandre Bonvin (1964) studied Chemistry at Lausanne University, Switzerland and obtained his PhD at Utrecht University in the Netherlands (1993). After two post-doc periods at Yale University (USA) and the ETHZ (CH) he joined Utrecht University in 1998 where he was appointed full professor of computational structural biology in 2009. In 2006, he received a prestigious VICI grant from the Dutch Research Council. He was director of chemical education (2009-2012), vice head of the Chemistry Department (2010-2012) and Scientific Director of the Bijvoet Centre for Biomolecular Research (2019-2023). He has and is participating to several EU projects including the BioExcel Center of Excellence in Biomolecular Simulations. His work has resulted in over 275 peer-reviewed publications.

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Solving 3D puzzles of biomolecular interactions by integrative modelling

Abstract

The prediction of the quaternary structure of biomolecular macromolecules is of paramount importance for fundamental understanding of cellular processes and drug design. In the era of integrative structural biology, one way of increasing the accuracy of modelling methods used to predict the structure of biomolecular complexes is to include as much experimental or predictive information as possible in the process. We have developed for this purpose the versatile integrative modelling software HADDOCK (https://www.bonvinlab.org/software) available as a web service from https://wenmr.science.uu.nl. HADDOCK can integrate a large variety of information derived from biochemical, biophysical or bioinformatics methods to enhance sampling, scoring, or both.

In my talk, I will highlight some recent developments around HADDOCK illustrating its capabilities with various examples including among others recent work on the modelling of antibody-antigen interactions from sequence only, a notoriously difficult class of complexes to predict for AI-based methods like AlphaFold2.

Ms. Jaya Panvalkar

Independent Director, Kinetic Communication Limited, Pune Ex Nvidia Pune center Founder and Head, Ex-Chairman, SVNIT, Surat

Profile

Ms. Jaya's career spanning 52 years in computer field, she has extensive 'make-in-India' contributions in prestigious CWPRS in domains of sea waves, earthquakes, soil and more. Jaya as CTO of PACE Soft Silicon became ISV and delivered for video recording/playback systems for camera phones. She instrumented acquisition of PACE by NVIDIA, and founded Pune Design Center as Site Leader. She spearheaded growth of PDC in technical leadership with 100+ patentable ideas, established 80+ Nvidia labs, technical forums. She served as Chairperson, BOD for SVNIT. Her contribution as Chairperson, HRD for National Supercomputing Mission are remarkable. She serves on Boards of industries.

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Transcending Technologies and Enablers

Abstract

In the last decade, High-Performance Supercomputing has made many scientists' lives a little easier by giving their hands the power of computing, reducing the time of research of many biological, microbiological, and bioinfo applications. At the same time, in the last 5 years, the era of Exascale computing has increased compute power multifold. Along with it, the revolution in the availability of vast amounts of data and algorithms which can use computer power for complex algorithms for ML, DL, Generative Artificial Intelligence (AI) and Intelligent Inferencing engines using General Purpose Graphics Processing Units (GPGPU) are invented by scientists. However, scientists are apprehensive about writing parallel programs using GPUs, as this involves relearning languages like CUDA and OpenAI to add parallel code snippets to the programs.

Computer scientists have solutions for everyone. They invented easy-to-use tools and APIs suitable for the application so that domain experts do not need to worry about programming and reprogramming. In addition, tools like Generative AI allow us to learn and improve the Inferencing iteratively, almost eliminating the need for training and retraining the app with newer data sets.

These new techniques and paradigms are useful for domain experts to apply their own applications in their domain without requiring programming expertise. This reduces dependency on programmers who do little or no programming. Isn't it nice?!!!

Shri Sanjay Wandhekar

Centre Head, C-DAC Pune

National Supercomputing Mission: Development of Supercomputing Ecosystem in the country

Abstract

The National Supercomputing Mission (NSM) has heralded a transformative era in India's technological landscape, orchestrated through a meticulously coordinated effort encompassing developers, users, academic institutions, and research centers. NSM has significantly boosted India's supercomputing capabilities by adopting a unique approach to the HPC infrastructure by executing three concurrent phases—Assemble, Manufacture, Design, and Manufacture—the mission has not only minimized redundancies but also optimized investments in supercomputing infrastructure. Indigenous development of hardware like the RUDRA Server boards and TRINETRA High-Speed Interconnects, as well as software initiatives enhanced efficiency and performance. Total computing capacity in India increased from around 10 PF in 2018 to over 80 PF by 2025 with approximately 64 PF attributed solely to NSM efforts. NSM Applications in the area of Genomics and Drug Discovery, Seismic Data Processing, Urban Modelling, Early Warning System, Computational Chemistry are available on NSM clusters and applications porting efforts have been put to tune it on NSM Rudra based clusters. All the research community across India have been benefited due to NSM. During pandemic, NSM supported hackathon for drug discovery as well as very large simulations efforts have been carried out to repurpose FDA approved drugs for Covid19. Ayurveda formulations for covid19 were also computationally tested for suitability using molecular docking, simulations and AI/ML data analytics. NSM has garnered international recognition, exemplified by C-DAC's affiliation with the Accelerated Data Analytics and Computing (ADAC) Institute and the US Government's proposal to elevate India's status from Tier 3 to Tier 1 country high-end in technology export restrictions. Recent collaboration with Euro HPC Centers of Excellence for development of advancing scientific and High-Performance Computing (HPC) applications has also been enabled due to NSM. Aligning seamlessly with the Government of India's vision of 'Digital India,' 'Make in India,' and 'Skill Development' initiatives, NSM stands as a beacon of innovation and progress in the nation's technological journey towards exascale computing.

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Session: Next Generation Drug Discovery, Repurposing and Toxicology

Prof. Andrew Lynn

Dr. Shanker Gupta

Dr. Ashwani Sharma

Prof. Andrew Lynn

Professor, School of Computational and Integrative Sciences(formerly known as School of Information Technology) Jawaharlal Nehru University, New Delhi

Hybrid Alchemical Free Energy/Machine Learning in the Design of Novel Lead Compounds from Fragment Seeds: Application to Cyclophilin Inhibitor Discovery

Abstract

Fragment-Based Drug Discovery (FBDD) leverages chemical fragments with moderate binding affinities to target proteins as building blocks for designing high-affinity lead compounds. Recent advancements in the drug discovery pipeline include alchemical free energy calculations to enhance the rescoring of potential inhibitors identified through virtual screening. However, these methods are computationally intensive and exhibit reduced accuracy when applied to smaller chemical entities such as fragments.

Machine learning (ML) offers a solution to these challenges by accelerating the evaluation of fragment-binding affinities and enhancing the predictive accuracy of free energy calculations. In this study, we present a computational pipeline that integrates ML to refine the prediction of fragment-binding free energies and to prioritize potential inhibitors through scaffold-hopping-based fragment linking.

Using cyclophilin as the target, a fragment library was initially screened via surface plasmon resonance (SPR) to identify binding fragments. Subsequent localization of these fragments within the target structure was achieved using nuclear magnetic resonance (NMR) spectroscopy, providing experimentally validated starting points for inhibitor design. This pipeline demonstrates the synergistic application of ML and alchemical methods in improving the efficiency and accuracy of FBDD, paving the way for the discovery of novel cyclophilin inhibitors.

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Dr. Shanker Gupta, Ph.D.

The Division of Cancer Prevention of National Cancer Institute, National Institutes of Health (NIH)

Profile

Dr. Shanker Gupta has over 25 years of experience in the pharmaceutical development of small molecules and biopharmaceuticals. Dr. Shanker Gupta is currently working in the Division of Cancer Prevention of National Cancer Institute, a component of the National Institutes of Health. His expertise is in the development and production of cancer vaccines – protein subunit, virus-based, DNA vaccines. Before joining Prevention Program, Dr. Gupta managed a diversified portfolio to produce vaccines and monoclonal antibodies for the Vaccine Research Center, NIH. His research interest is in the development of mRNA-based cancer vaccines. He has numerous patents in formulation development and has published in peer-reviewed journals.

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Quadrivalent Lynch Syndrome Vaccine Product Development

S. Gupta,[1] R. Shoemaker,[1] Timothy Fouts[2] and Indu Javeri[3]
[1]CADRG-[1], Div Cancer Prevention, NCI [2]ABL, Inc., Rockville, MD.
[3] CuriRx, Wilmington, MA.

Abstract

A stable lyophilized formulation for a cancer vaccine containing the quadrivalent frameshift peptides (FSP) AIM2(-1), HT001(-1), and TAFB (-1), TGFBR2(-1), was obtained through an iterative screening process. To develop a lyophilizable formulation, the screening included evaluation of pH, stabilizers, bulking agents, and surfactants. The screening resulted in a scalable formulation and lyophilization process with 100 μg/ml each peptide,10 mM Histidine at pH 5.5, 260 mM trehalose, and 0.02% polysorbate 20 as a lead formulation. Based on peptide content and peptide purity from a three-month stability study, the lead lyophilized formulation is estimated to be stable at refrigerated temperature for more than 2 years.

Dr. Ashwani Sharma

Associate Professor, Department of Chemistry & Biology, IISER Tirupati

Profile

Dr. Ashwani Sharma completed his PhD in 2011 from National Chemical Laboratory (NCL), Pune. He did his post-doctoral studies from University of Utah and Markey Cancer Centre, University of Kentucky, USA from 2011–2015. After coming back to India, he joined as DST young scientist in Indian Institute of Chemical Technology (IICT), Hyderabad for a short span of one year. He joined IISER Tirupati as an Assistant Professor in 2017 and promoted to Associate Professor in 2023. His area of interest is RNA biology. His lab work on RNA nanotechnology for targeted drug delivery, developing RNA aptamers, ribozymes and utilizing them in the detection of small molecules as well as macromolecules. His lab is also interested in RNA engineering for efficient gene editing, and to understand the role of various non-coding RNAs in the cell.

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Engineering RNA junctions for better stability and functionA. Murali Krishna and Ashwani Sharma*

Abstract

RNA has the ability to fold into complex secondary structures involving various structural motifs such as loops, stems, junctions including three-way junction (3WJ), four-way junction (4WJ) etc. Stability of these junctions are fundamental to RNA folding that relates to the RNA function. Many highly stable naturally occurring RNA motif exists that are important for RNA folding and function. For instance, packaging RNA three way junction motif (pRNA-3WJ) in pRNA from Phi-29 bacteriophage that packages viral DNA to its capsid is known to be highly stable natural RNA 3WJ motif. The motif has been used intensively to construct boiling resistant highly stable RNA nanostructure for drug delivery applications.1

However, there are no high throughput ways to engineer new RNA junctions by changing individual nucleotides. We present here a simple fluorescence based strategy using light-up aptamers to screen engineered RNA motifs. The stability of these engineered RNA motifs would depend on the fluorescence output of light-up aptamer. Using this strategy, we were able to engineer a less stable 5S-3WJ motif to a more stable 5S1-3WJ motif. We further hypothesized that the new highly stable engineered junctions would be helpful to fold an RNA into the desired conformation out of all other possible conformations, and thus would lead to enhanced RNA functionality. Engineered RNA motifs were introduced to few functional RNAs that lead to enhanced functionality. Highly stable engineered 3WJ motifs were also used to construct various 2D and 3D RNA nanostructures for drug delivery applications. The thermal and enzymatic stabilities of 3WJ, and constructed nanostructures were also compared.

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Session: Biomarker Discovery in Genomics

Dr. Sanjay Gupta

Prof. Mukesh Jain

Prof. Shandar Ahmad

Dr. Akash Ranjan

Dr. Sanjay Gupta

Professor, Translational Research and Principal Investigator, Gupta Lab, ACTREC, Tata Memorial Centre, Mumbai

Profile

Dr. Sanjay Gupta was awarded his Ph.D. from the Banaras Hindu University, Varanasi, in 1995 in the area of aging, chromatin biology, and gene regulation. Following his Ph.D., he had a short stint as a visiting research associate at the Institute of Life Sciences, Bhubaneswar, followed by post-doctoral and DST-young scientist fellowships. He joined the Cancer Research Institute, Tata Memorial Centre, Mumbai, in 1999. Prof. Gupta has significantly contributed to the field of epigenetics, specifically on histone isoforms and variants, their site-specific post-translational modifications in cancer pathogenesis, resistance, and cell-cycle-specific DNA repair mechanisms. Moreover, he is deciphering the importance of epigenetic mechanisms in regulating gene expression in cancer. His group exploits these epigenetic changes for biomarker development and epi-drugs for therapeutic potential in cancer. Dr. Sanjay has published several peer-reviewed research papers in national and international journals. He serves on national and international committees like SERB-DST, HPC-Ministry of Electronic and IT, and UICC. He is the Associate Editor of the Journal of Integrated–Omics, A methodological journal, an Editorial Board Member of the Journal of Clinical Epigenetics, and an Associate Editor of the Journal of Radiation and Cancer Research. A database, HISTome2 (https://www.actrec.gov.in/histome2/), was developed for histone proteins and epi-drugs on one interface.

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Biomarkers And Their Effect On Personalized Cancer Treatment: The Connection Between Cancer Epigenetics And Metabolism

Abstract

Precision or personalized therapy is replacing the "one size fits all" approach to cancer treatment. The identification of biomarkers for their possible application in the clinical management of the disease was prompted by the altered molecular pathways, genetic, epigenetic, metabolic, and signaling, linked to cancer growth, progression, and resistance mechanisms. The group's ongoing research has demonstrated that metabolic reprogramming occurs in cancer and resistance mechanisms, suggesting that cancer cells have regulated metabolic plasticity. Furthermore, epigenetic modifications affecting gene transcription and phenotype are closely linked to metabolic changes. Thus, investigating the processes behind epigenetic changes that control the reprogramming of tumor cell metabolism is essential to comprehending early-cause tumor pathophysiology and recognizing probable treatment avenues. The talk will cover cell metabolism and epigenetic changes in the context of cancer and resistance mechanisms before emphasizing the potential combination of targetable biomarkers to promote precision medicine for therapy.

Prof. Mukesh Jain

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

Profile

Dr. Mukesh Jain is currently serving as a Professor at the School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi, India. He has worked extensively in the areas of Plant Genomics, Biotechnology, and Computational Biology. He is one of the pioneers of next-generation genomics research in plant sciences in India. For his outstanding scientific contributions, Prof. Jain has been honored with several awards and Fellowships of the National Academies.

Dr. Jain's current research interests include understanding epigenetic and chromatin-level regulation of abiotic stress responses and seed development in crop plants using integrated multi-omics, single-cell genomics, and systems biology approaches.

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Integrated omics approaches for divulging molecular signatures associated with agronomic traits

Abstract

Next-generation sequencing (NGS) technologies provide a revolutionary tool with numerous applications. Further, advances in multi-omics approaches have accelerated efforts for gene discovery and understanding the molecular basis of important agronomic traits for undertaking translational research. I shall illustrate the use of NGS technologies in generation of genomic resources and connecting genes and genomic variations to agronomic traits giving examples from a non-model (chickpea) crop plant. We sequenced the genome/transcriptome of chickpea to reveal the gene space and genetic variations associated with important agronomic traits. A comprehensive analysis of transcriptome dynamics during seed development in two chickpea cultivars with contrasting seed size identified a significant proportion of the genes exhibiting stage- and cultivar-specific expression patterns. The transcriptional changes in cell cycle, endoreduplication, carbohydrate metabolism and hormone signal transduction pathways were found to determine seed size/weight in the chickpea cultivars. Further, we revealed the regulation of candidate genes via differential DNA methylation and non-coding RNAs. In addition, we have developed a comprehensive gene expression atlas and demonstrated its applications in functional genomic studies and candidate gene discovery. Our studies provide insights into the molecular signatures and regulatory mechanisms underlying agronomic traits and will surely facilitate research in various areas of functional and translational genomics in crop plants.

Prof. Shandar Ahmad

Professor and Coordinator (DBT-Bioinformatics Centre), School of Computational and Integrative Sciences (SCIS), Jawaharlal Nehru University (JNU), New Delhi

Profile

Dr. Shandar Ahmad is a Professor and Coordinator of DBT-Bioinformatics Centre and also a former Dean of the School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi. Earlier, he has worked in National Institute of Biomedical Innovation, Health and Nutrition, Japan (2007-2016), where he still holds an honorary Visiting Scientist position. He was also an adjunct Associate Professor at Graduate School of Frontier Biosciences, Osaka University (2008-2016). He is in the Editorial board of BMC Medical Genomics, BMC Artificial Intelligence and Frontiers in Bioinformatics and is currently appointed as Editor for a Special Issue on protein-nucleic acid interactions for Current Opinions in Structural Biology.

Shandar Ahmad developed the first machine learning methods for sequence-based prediction of DNA-binding sites and first regression model to predict solvent accessibility in proteins way back in 2004. His lab called SciWhyLab continues to make significant contributions to the study of sequence and structural analysis of protein-DNA and other bio-molecular interactions, particularly their modeling through conventional and deep machine learning. They have developed a method to infer nucleic acid-sensing behavior of toll-like receptors from sequence, structure and network features. SciWhyLab is also interested in developing transcriptome-based methods for drug discovery (TBDD) and integrating them with traditional structure based approach (SBDD), whole organization of of bacterial and human genomes and functional genomics involving sequence-dependent DNA shape and dynamics including HiC-inferred chromatin structures.

Most recent advances of the lab include a though integration of global gene expression data sets and pan-cancer models for predicting drug sensitivity in PDX models, and the first ever (experimental and computational) determination of HiC structure of MTB genome.

For more, visit his website www.sciwhylab.org

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AI-driven integrative and alternative Biomarkers: Cross-platform transcriptomics and the genomic language of DNA-shape

Abstract

In this talk, I will highlight two alternatives to conventional biomarker-based characterization of cellular states. First, we will present the use of whole transcriptome and their universal subsets, which are a step in the direction of universal biomarkers and the other is the dictionary-based approach to
represent conformational space of DNA short sequences, which describes the DNA-shape alphabet of genome. I will discuss, specific systems on which these approaches are showing promising success including application to Trancriptome based drug discover (TBDD).

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5. Unpublished works

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Accelerating disease biology research: Unravelling the mechanistic connection between biomarker mutations and genetic diseases through computational approaches

Abstract

Among human diseases, rare genetic diseases are a class of chronic, debilitating disorders that have not received sufficient attention in terms of diagnosis, research, and therapeutic development. Of the estimated 350 million individuals worldwide afflicted with rare genetic diseases, India is home to approximately 70 million. Further, there are likely to be many genetic disease patients who show associative mutations with unexplained genetic/mechanistic bases. These mutations can have wide-ranging adverse consequences on protein production, folding, stability, subcellular localization, protein-protein interaction, complex formation, and function. In some cases, these mutations can contribute to causing rare genetic disorders in humans. In this direction, our group is a part of the DBT Mission program on Paediatrics Rare Genetic Disease, which aims to identify the molecular mechanisms through which genetic mutations can cause disease and explore potential therapeutic interventions and strategies for the disease. This program is a multicenter program that takes an integrated approach to studying Paediatrics Rare Genetic Diseases. In this program, our goal is to understand how mutations cause disease by altering protein structure and function. Specifically, we aim to elucidate the molecular mechanisms by which mutations lead to disease. This is likely to pave the way for precision medicine for the disease.

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Session: Empowering Molecules: Multiscale Simulations

Prof. Sanjib Senapati

Prof. B. Gopal, IISc

Prof. Aditya Mittal

Dr. Chetan Gadgil

Prof. Sanjib Senapati

Professor and Head, Dept. of Biotechnology,
BJM School of Biosciences, IIT Madras, Chennai

Profile

Dr. Sanjib Senapati is currently a Professor and Head of the Dept. of Biotechnology, IIT Madras, where he is working since 2006. Prior to this job, he was a Research Scientist in the Dept. of Chemistry and Biochemistry, University of California, San Diego, USA, 2003 – 2005 AND a Post Doctoral Fellow in the Department of Chemistry, University of North Carolina, Chapel Hill, USA, 2001 - 2003. He obtained his Ph. D. degree in Theoretical Chemistry from Indian Institute of Technology, Kanpur, India in the year 2001. His research is focused on Computational Biology Molecular dynamics simulations of proteins and protein-ligand complexes, Computational Chemistry Green solvents for dissolution and improved stability of DNA and proteins, In-vitro verifications of computational findings. Dr. Sajib has been awarded Fulbright-Nehru Academic and Professional Excellence Fellowship 2016, National Bioscience Award 2015, DBT, Govt. of India and NASI-SCOPUS Young Scientist Award in Biological Sciences, 2011, Scopus, South Asia. He has published more than 100 research articles in top-tier journals like JACS, Nucleic Acids Research, Journal of Biological Chemistry, Physical Review Letters, Biochemistry, Soft Matter etc.

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A multiscale computational approach to identify novel viral epitopes by targeting MHC-TCR complexation

Abstract

T-cell immunity is a crucial defense against viral infections in vertebrates. Upon viral entry, innate immune cells process viral proteins and present them via Major Histocompatibility Complex (MHC) molecules. T-cell receptors (TCRs) recognize these MHC-bound viral peptides (pMHC), initiating a T-cell-mediated immune response. Despite its significance, the mechanism by which pMHC-TCR binding triggers T-cell activation remains unclear. This study integrates Molecular Dynamics (MD) simulations and machine learning (ML) approaches to predict viral epitopes as vaccine candidates. We performed large-scale all-atom and coarse-grained MD simulations on MHC-peptide-TCR complexes embedded into dendritic and T-cells, respectively, starting from the available experimental immunogenicity data. One hundred twenty such systems are simulated for 1 □s each to capture the conformational and dynamical changes that underlie T-cell activation. Machine learning models developed over the simulation data provide insights into the conformational changes responsible for T-cell activation. We have identified key features influencing immune response, including the bending of the TCR alpha membrane region and the exposure of buried surface area between the pMHC and TCR, among others. Our approach would advance the understanding of T-cell immunity and accelerate the screening of viral epitopes for vaccine development.

Prof. B. Gopal

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Profile

B. Gopal is a Professor at the Division of Biological Sciences, Indian Institute of Science, Bengaluru. An alumnus of the Maharashtra Education Society, Pune, Indian Institute of Technology, Kanpur and Indian Institute of Science, Bengaluru, he is structural biologist by training. His current research interests include gene expression analysis and synthetic microbiology. In addition to his academic affiliation, he has been associated either as a co-founder, advisor or consultant to start-up and mid-size biotechnology and pharmaceutical industries involved in the production of biosimilars and active pharmaceutical ingredients. He is a fellow of all three science academies in India and a recipient of the Shanti Swaroop Bhatnagar prize awarded by the Council for Scientific and Industrial Research, Government of India.

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Simulation-guided engineering of Escherichia coli for bioprocessing applications

Abstract

Escherichia coli is an important production host to produce fine chemicals as well as therapeutic products. Traditionally, E. coli K-12 and B strains have served as chassis for synthetic biology programs. However, both strains and their derivatives produce high levels of acetate, an undesirable by-product formed during anaerobic fermentation, leading to reduced cell growth. We present simulation-guided engineering of E. coli W that can grow on sucrose containing media and can potentially overcome the limitations of both E. coli K-12 and B strains. Alongside gene deletions or insertions guided by simulations and flux analysis, we utilize information on the altered transcriptional and translational patterns to deploy synthetic Extracytoplasmic function (ECF) σ factors to calibrate target gene expression. Structural studies reveal that promoter specificity in a σ factor is determined by the interactions between a loop (L3) and the Pribnow box element. The efficiency of transcription initiation is governed by a polypeptide linker between the two promoter binding domains. Both these polypeptide segments are dynamic and poorly conserved amongst ECF σ factor homologues. We describe an approach to characterize these features that govern the dynamic range of gene expression using chimeric E. coli σE. The L3 loop and linker polypeptides in these σE chimeras were replaced by the corresponding segments from ten annotated and functional M. tuberculosis ECF σ's. In vitro and in vivo measurements to determine the effect of these polypeptide replacements provided an experimentally validated σE chimera- gene expression level dataset- information that could potentially feed into simulations. We illustrate the build-test-learn utility of this chimeric σE library in improving the efficiency of a biosynthetic pathway in *E. coli.*

Prof. Aditya Mittal

Professor and Dean, Student Affairs,
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Indian Institute of Technology Delhi, New Delhi

Profile

Prof. Aditya Mittal received his B.Tech. in Biochemical Engineering from HBTI, Kanpur, India (1996), after which he worked as a Brewer with Shaw Wallace & Co. (1996-1997) where he was involved in production of the then leading beer brands of India – Royal Challenge, Haywards 5000 and Haywards 10000. Subsequently, he earned his Ph.D. in Biological Sciences from Drexel University, Philadelphia, PA, USA (2002, Field: Membrane Biophysics, Area: Viral Fusion Mechanisms). Additionally, at Drexel, he worked on drug transport by the multi-drug resistance protein MDR1 in collaboration with Glaxo-SmithKline, and, was involved in synthesis of gold/silver nanoparticles and nanowires using a contact-less method called SCBE at the Dept. of Chemistry. He then worked as a Visiting Fellow at the National Institutes of Health (NIH), Bethesda, MD, USA on remodeling of biological membranes. He joined IIT Delhi in 2004 as an Assistant Professor to set up his independent research program exploring kinetics and self-assembly in biological systems. In 2008 he was approached to serve as a founder faculty member of the School of Biological Sciences at IIT Delhi for popularizing modern biology amongst UG students, while developing vibrant post-graduate programs in biology. He was one of the youngest at IIT Delhi to be selected as a full Professor and subsequently being granted the HAG-scale. He continues to conduct and publish his research based on his interests, often considered esoteric for 'classical biology'. He was honored as an Associate of the Indian Academy of Sciences and was featured in the cover story of a 2006 issue of Chemical & Engineering News (American Chemical Society) as one of five Indian scientists in the section "India's Young Blood". He was also designated as "Asia21 Young Leader" by the Asia Society, New York, USA in 2006. He has served/serves as an Editor/Editorial Board Member for scientific journals in both applied and basic biological sciences, and serves as reviewer in several top multi-disciplinary journals. He has also Chaired/served-on several national and international committees on research and education. He has guided/supervised several post-graduate theses (doctoral and masters) and under-graduate projects, many of which have led to the students receiving national and international awards. In 2015, a Teaching Excellence Award was conferred on him by IIT Delhi. Aditya's pioneering research on bacterial nanomagnets was recognized by DST with certificates of excellence. Amongst millions of living species on Earth, only 50 "chemical formulae" for living organisms have been discovered. Aditya's work is the only one from India to be a part of this elite group. He also formulated the "Stoichiometry-Driven Protein Folding" hypothesis along with his friend and colleague B. Jayaram. Having been invited/selected to serve as faculty in the Department of Biochemical Engineering and Biotechnology, and the Center for Biomedical Engineering, he also served as a founder of the School of Biological Sciences at IIT Delhi. He continues to contribute to engineering education via several National responsibilities. As the Chairman of JEE (Advanced) 2018 at IIT Delhi, he co-organized (with IIT Kanpur) the first Computer-Based-Test for undergraduate admissions to 23 IITs. Having played a key role in successfully defending the IIT system in the Hon'ble Supreme Court of India (01 case) and several Hon'ble High Courts in the country (17 cases), one of his appearances in the Hon'ble High Court of Delhi was anecdotally recorded as "Prof. Aditya Mittal, Advocate" in the judgment. Recently, he completed his tenure as the Dean, Student Affairs at IIT Delhi and was appointed as a member of a High-Level Committee of (seven) Experts on reforms in National Examinations formed by GoI (subsequently endorsed by the Hon'ble Supreme Court of India).

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Implications of Stoichiometric Compositions on Order and Disorder in Natural Proteins

Abstract

More than a decade ago, rigorous analyses of structural data of thousands of naturally occurring folded proteins yielded a "margin of life" for stoichiometric composition, i.e. percentage occurrence of individual amino acids, of protein sequences (Mittal et al., 2010; Mittal and Jayaram, 2011a, 2011b). This "margin of life" refers to the lower-than-expected variances in percentage occurrence of individual amino acids in protein sequences (Mezei, 2011). Subsequently, the constraints on stoichiometric compositions have been confirmed over a large sequence space for almost all known protein sequences (even in absence of structural data). While the earlier work was based on the largest structural dataset at that time (several thousands of structures), in this talk further explorations on compositional considerations for known protein sequences will be discussed. The relationships between occurrences of all possible di-, tri-, tetra- and penta- peptides, in more than half-a-million curated (manually annotated and reviewed) primary sequences, with their various physico-chemical properties and individual proportions of amino acids will be explored, while reporting the fascinating discovery of a tetra-peptide 'CQWW' absent from naturally occurring proteins (Mittal et al., 2020, 2021a, 2021b). A key result conclusively shows that stoichiometric constraints on amino acids limit the primary sequence space of proteins in nature rather than any perceived limitations of evolutionary sampling of the primary sequence space for natural occurrence of proteins. There are profound evolutionary implications (Mittal and Chauhan, 2022) of our insights into occurrence of naturally occurring protein sequences, especially in the context of functional, stable and structurally controlled and/or "disordered" flexible proteins.

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Dr. Chetan Gadgil

Scientist and Head, Chemical Engineering Division, CSIR-NCL, Pune
Dean, Engineering Sciences, AcSIR

Profile

Dr. Chetan Gadgil studied Chemical Engineering at UDCT Bombay, IIT Bombay and the University of Minnesota. After his PhD he was a postdoctoral researcher in the Mathematics department at the University of Minnesota. He then worked in the US-based R&D division of the pharmaceutical company GlaxoSmithKline (GSK) before joining NCL Pune as a scientist. His research group works on application of mathematical modelling and data analysis to biological systems at scales ranging from individual reactions to pharmacology. He has also contributed to academic evaluation and administration, as a member of several SERB, BIRAC and DBT committees, as the Head of the Chemical Engineering and Process Development Division at NCL, and currently as Dean (Engineering) in AcSIR.

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Understanding the building blocks of biological processes

Abstract

For most decision-making with large irreversible consequences, it is important to understand the outcomes of computation. Through two examples of such 'compute to understand', we show how old-fashioned pen-paper calculations and simulations shed light on biological processes at two different scales: enzyme inhibitors and memory. In the first example we show how for competitive (but not uncompetitive) inhibitors, the inhibitor effect on the initial rate of product formation is qualitatively different than the effect on steady state product levels. Interestingly, for reversible enzymatic reactions, competitive inhibitors counterintuitively increase the steady state product concentration relative to the uninhibited reaction product. In the second example, we show how 'simple' motifs are capable of generating responses similar to that of learning and memory, where the spacing between training sessions dictates the extent of information retained. We test this result using an existing model for long term potentiation, where we show that individual arms of the feed-forward network are sufficient to generate an inverted-U response to increase in inter-stimulus interval.

Session: Computational Applications in Traditional Medicine

Prof. B. Jayaram

Dr. Debasisa Mohanty

Dr. Kuldeep R. Choudhary

Prof. B. Jayaram

Emeritus Professor, Department of Chemistry & Kusuma School of Biological Sciences, Co-PI & Mentor, Supercomputing Facility for Bioinformatics and Computational Biology (SCFBio), IIT New Delhi

Profile

Prof. B. Jayaram is currently Mentor, SCFBio, IIT Delhi. Prof. Jayaram received his Ph.D. in 1986 from the City University of New York, USA. He then worked as a Post Doctoral Fellow at Columbia University, NY, USA and as a Senior Research Associate at Wesleyan University, CT, USA. In 1990, Prof. Jayaram joined IIT Delhi and worked as a Faculty at IIT Delhi (1990-2023), as Head of Chemistry Department, IIT Delhi (2006-2009), as Founder Coordinator of the Kusuma School of Biological Sciences, IIT Delhi (2008-2014), and as Founder Coordinator of the Supercomputing Facility for Bioinformatics & Computational Biology (SCFBio), IIT Delhi (2002-2019). He guided 30 PhD students (28 completed and 2 in progress) and dissertations of over 150 M. Tech., M.Sc. and B. Tech. students. Prof. Jayaram was responsible for the creation of the science and software of the Dhanvantari (Genom ?Gen ?Protei ?Drug pathway) suite and several other molecular modelling and bioinformatics utilities, and making these software tools freely accessible to the global user community through SCFBio website. During this scientific journey, Prof. Jayaram with his students and colleagues made several important discoveries of relevance to bimolecular function. One was the conjugate rule among nucleic acid bases which explained degeneracies in genetic code and paved the way for a physico-chemical approach to genome annotation. This was followed by their discovery that energetic and structural properties of DNA sequences conveyed their functional destiny as demonstrated by them for gene, promoter, intron-exon boundary detections. Most notably, sequence to structure and dynamics to function was an established axiom in protein science. Their studies demonstrated that this axiom was true for nucleic acids as well. On the protein front, they discovered that just four physico-chemical properties of amino acids not only explained the existence of the magic number 20 for naturally occurring amino acids, but also set very high water mark for homology modelling and function prediction. They also found that millions of proteins chronicled till date shared a similar stoichiometry with very small standard deviations in their amino acid compositions which they called as the margin of life. Equally interesting was the observation that there was a universality in the spatial distribution of the C-alpha atoms for any pair of amino acids. They also demonstrated that higher order Ramachandran maps carried sufficient information to build tertiary structures. Their analyses of the configurational space of proteins suggested, when higher order spatial correlations of amino acid residue neighbours were included, that protein folding was a convergent problem as opposed to the then conventional wisdom. Alphafold has now proved it. The Sanjeevini software they built for computer aided drug discovery, is comprised of several new methods for active site detection, docking and rapid screening of large libraries of small molecules etc.. Sanjeevini software suite has already delivered experimentally validated molecules against HAV, HBV, CHIKV and fungal infections, breast cancer and malaria.

Prof. Jayaram served as a Member/Co-chair of several technical committees of DST, DBT, MEITY of Govt. of India, IUPAB National Committee and Indian Biophysical Society over the years. He published over 150 papers in peer-reviewed international journals and delivered over 300 invited talks. Please visit http://scfbio-iitd.res.in/BJ_SCFBio_Web_2024.pdf for details.

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Harnessing Indian Medicinal Plants as Sources of Potential Therapeutic Agents

Abstract

The historical importance of Indian medicinal plants is well documented in traditional systems of medicine. These plants are renowned for their medicinal effects that enhance general well-being. With modern scientific progresses, there has been an increased interest in exploring the bioactivity of these plants to uncover the active compounds responsible for their pharmacological effects. In this context, a manually curated database called BIMP (https://scfbio.iitd.ac.in/bimp) is introduced here. This database provides information on 105,909 Phytochemicals found in 6,209 Indian medicinal plants. It includes information on both known and predicted targets for the compounds, along with specifics on the diseases and the target genes/proteins with information of organisms. RASPD+ (http://www.scfbio-iitd.res.in/raspd+/index.php) is a tool available at SCFBio, which rapidly identifies molecules for a specified target and FishBait (http://www.scfbio-iitd.res.in/fishbait/about.php) is another tool from SCFBio which identifies protein targets for a bioactive molecule. Together, BIMP, RASPD+ and FishBait can accelerate drug discovery efforts. The talk will present BIMP database with a couple of case studies.

Reference:

Dheeraj Kumar Chaurasia, Raushan Anjum, Aman Sharma, Shashank Shekhar, Ashok Kumar Patel, Aditya Mittal, and B. Jayaram, "BIMP: Unveiling the Phytochemical Richness of Indian Medicinal Plants as Potential Therapeutic Agents", submitted, 2024.

Dr. Kuldeep R. Choudhary

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Profile

Dr. Kuldeep R. Choudhary is M.D. in Ayurveda Pediatrics from the National Institute of Ayurveda, Jaipur (Deemed To be University (De Novo) Ministry of AYUSH, Govt. of India). He is presently working as a Research officer (Ayurveda) in CCRAS, Ministry of Ayush, Govt. of India since 2017, currently posted at RRAP – Central Ayurveda Research Institute, Mumbai. He is the Group Coordinator of the Focus group of CCRAS for Research in RCH with a main focus on Pediatrics. His research area of interest is in Pediatric integrative oncology and Neurodevelopmental disorders.

Along with the clinical and teaching experience of more than 15 years, as a Researcher, he is currently working on 6 projects as Principal Investigator and 3 projects as Co-Investigator. He has completed 6 projects as Principal Investigator, and 5 as Co-investigator. He was involved in clinical and research work on COVID-19. Notably, projects on AYUSH 64 in mild to moderate COVID-19 patients and Ashwagandha as prophylaxis against COVID-19. He has more than 22 scientific publications in peer-reviewed national and international journals. He is a reviewer for PLOS one, JAIM (Journal of Ayurveda and Integrative Medicine), AYU Journal (An International Quarterly Journal of Research in Ayurveda) and the Journal of Ayurveda (Medknow Publications).

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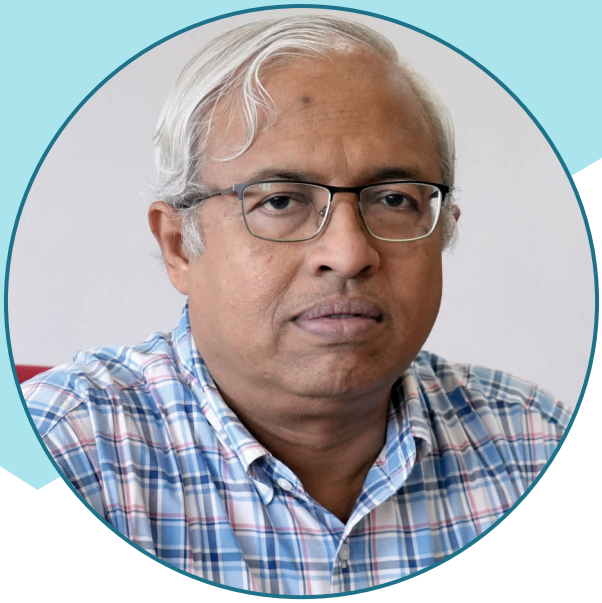
Leveraging Computational Tools, Material Basis Approach for Advancing Ayurveda Therapeutics

Abstract

Indian Traditional medicine systems, such as Ayurveda, Yog, Siddha, Sowarigpa, and Unani, have a rich history of holistic healthcare practices. With the advent of computational technologies, there is a growing opportunity to integrate these ancient systems with modern scientific methods to enhance their efficacy and accessibility.

For all pragmatic purposes, the material basis approach forms the crux of understanding Ayurveda, which employs complex natural substances for various interventions. To decipher the holistic material basis, there is a need to transition from examining isolated bioactive entities to understanding their synergistic interactions, which are anchored by three pivotal elements—chemical structure, stoichiometric structure, and aggregate structure.

This presentation explores the application of computational tools, including artificial intelligence (AI), machine learning (ML), data mining and the Material Basis approach for the understanding of Ayurvedic therapeutics with the following goals: Improved diagnostic accuracy and Personalization of treatments, improving crosstalk between practitioners of Ayurveda, biomedicine and develop safe and effective integrative treatment approaches for refractory, non-communicable diseases. By bridging the gap between traditional wisdom and modern computational techniques, we aim to unlock new possibilities for advancing healthcare and preserving the valuable heritage of traditional medicine.



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New Delhi

Profile

Dr. Debasisa Mohanty completed his M.Sc. degree in Physics from IIT Kanpur in 1988 and carried out Ph.D. in computational biophysics from IISc, Bangalore. After completion of Ph.D. in 1994, Dr. Mohanty went abroad for postdoctoral training at Hebrew University of Jerusalem, Israel and Scripps Research Institute, La Jolla, USA. Dr. Mohanty joined NII, New Delhi in 1998 to lead a research group in Bioinformatics and Computational Biology. His research at NII is focused on development of structural bioinformatics and atomistic simulation methods for analysis of protein-protein and protein-nucleic acid interaction networks and in silico identification of novel biosynthetic pathways. Dr. Mohanty was appointed as Director of NII, New Delhi on 24th August 2022. Dr. Mohanty is a fellow of NASI, IASc & INSA, member of Guha Research Conference (GRC), recipient of National Bioscience Award, Rajib Goyal young scientist prize in life science and Samanta Chandrashekhar Award (Govt. of Odisha). He is currently chairperson of the Technical Expert Committee (TEC) of DBT, India for Theoretical & Computational Biology, member of INSACOG-SCAG and member of several other TECs of DBT and MeiTY.

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Recent advances in AI/ML based methods for prediction of structure, dynamics and ligand binding affinity of proteins

Abstract

Recent availability of deep learning and LLM-based methods, such as AlphaFold, RoseTTAFold, ESMFold etc has significantly advanced structural biology by offering novel solutions to the protein folding challenge as well as in the prediction of protein complexes. Machine learning has also helped in deciphering conformational transitions. This opened up opportunities for developing ML-based scoring functions for binding affinity prediction based on training on available datasets of crystal structures of protein-ligand complexes with known binding affinity values. Nevertheless, there remains a need to investigate the benefits and limitations of current machine-learning methods. The talk will give an overview of the advances and evaluate the performance of AI/ML methods like AlphaFold and the language model-based ESMFold on protein sets lacking suitable templates. In addition, advances in development of novel ML-based scoring function for binding affinity prediction will also be discussed.

Session: Ideas to Impact

Prof. Binay Panda

Dr. Mahesh Dharne

Dr. Samiron Phukan

Dr. Deeksha Bhartiya

Prof. Binay Panda

Professor, School of Biotechnology & Special Centre for Systems Medicine (Concurrent Appointment), Jawaharlal Nehru University, New Delhi

X-plat: a cross-platform transformation tool based on the nearest neighbor joining framework

Abstract

The biological data deluge using high-throughput tools, like microarrays and sequencing, has defined biology and medicine in the last decade. However, finding biological and clinical relevance using tools of genomic medicine from this large amount of data will require building robust algorithms to integrate molecular data with functional, clinical, and epidemiological information in a multi-modal and multi-dimensional context. Combining data from legacy microarray platforms and high-throughput sequencing platforms via discovery and validation of results will significantly benefit data validation. This is especially important in clinical domains where retrieving samples from deceased individuals is impossible. However, incompatibility among technologies due to design considerations, target preparation, and dependence on prior annotations makes legacy data unusable. Here, we describe a cross-platform data transformation tool, X-plat, that works both for expression and methylation data and inter-converts data for comparison between platforms without compromising throughput. X-plat builds a per-gene predictive model by connecting the nearest neighboring data points using a nearest neighbor-joining (NNJ) framework, followed by Root Mean Square Error (RMSE) minimization. In its subsequent iterations of the algorithm, X-plat builds transformation rules for clusters of genes with lower RMSE over individual genes, thus reducing the model size and compute time. X-plat used the cross-platform conversion rules discovered and validated using paired mixed source microarray: sequencing gold standard datasets across conditions, sources, and diverse organisms. I shall present data on X-plat, which outperforms other published normalization and conversion tools, such as harmony, distran, dwd, gq, mrs, qn, and tdm. Currently, we are building an easy-to-use graphical user interface (GUI) with X-plat for end-users.

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Dr. Mahesh Dharne

Senior Principal Scientist and Head
National Collection of Industrial Microorganisms
(NCIM) CSIR-National Chemical Laboratory,
Pune

Profile

Dr. Mahesh Dharne is currently working as Senior Principal Scientist in Biochemical Sciences Division at CSIR-National Chemical Laboratory, Pune, India. He is a Microbiologist by training and presently heading India's one of the oldest microbial repository i.e. National Collection of Industrial Micro-organisms (NCIM). NCIM is engaged in supply of microbial strains supply to various industries and academia. His research group uses cutting edge technology of next gen sequencing for addressing important questions in the field of Microbiology. His group has been pivotal in understanding environmental microbiome of various niches including Ganges river, mula-mutha river, lonar lake and understood the plethora of microbiome related to antimicrobial resistance. His team has significantly contributed in environmental surveillance of SARS CoV2 during covid-19 pandemic, which largely helped to mitigate the surveillance efforts in Pune and also Maharashtra state. Efforts are also underway to implement environmental surveillance strategy as a policy in hospitals and One health sector while paving path for Viksit Bharat by 2047.

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Environmental surveillance coupled with genomics for pathogen monitoring as an early warning system; a hope for pandemic preparedness?

Abstract

Environmental surveillance offers a population-level perspective by analyzing viral particles shed in sewage. This approach is particularly valuable because several viruses, including SARS-CoV-2, are excreted in feces by both symptomatic and asymptomatic individuals. By detecting viral signatures in wastewater, WBE complements traditional methods and potentially offers earlier warnings of outbreaks by providing insights into community transmission patterns. It has successfully detected genetic material from enteric viruses, tracked the re-emergence of zoonotic hepatitis E virus, and contributed to poliovirus eradication efforts. By November 2020, we successfully detected the coronavirus fragments in the sewage water. In January 2021, traces of new variant called double mutant (later named as Delta) was observed in genome sequencing of the sewage samples. This led to delta wave. Given the success of pilot project, a larger study was supported by Rockefeller Foundation, USA to expand sewage surveillance into 4 cities in India- Pune, Bangalore, Hyderabad, and Delhi under the Alliance for Pathogen Surveillance Innovation (APSI). This involves regular monitoring of viral and bacterial pathogens from sewage water by the participating local research laboratories and government bodies. Under this study, 10 Sewage treatment plants from Pune were analyzed covering 92% of the city's population. In late December 2021, increased viral load in sewage indicated potential new variant- i.e. omicron was detected just before the beginning of the third wave and the clinical tests. The sewage surveillance data is regularly shared with the health department, Pune Municipal Corporation- to the Mayor and Chief Executive Officer, Maharashtra COVID Task Force. By the end of December 2023 and early January 2024, a new variant of coronavirus called KP.2 was detected in Pune's wastewater samples of STP and of hospital, months before it was observed in the clinical samples in mid January 2024. This collaborative work is published in the Journal of Travel Medicine in July 2024 issue. Similarly, we are also addressing antimicrobial resistance in Pune wastewater using metagenomic and culture based analysis.

Dr. Samiron Phukan

Sr. Director, Integrated Drug Discovery
Aragen Life Sciences Ltd, Hyderabad

Profile

Dr. Samiron Phukan has over 20 years of experience in the field of computer aided drug design & AI/ ML driven solution in drug discovery and development. He had worked in various pharmaceutical companies and CROs in India in the field of drug discovery and development from concept to clinic. He had successfully delivered leads and clinical candidates in various therapeutic areas like oncology, metabolic disorders and anti-infectives. Presently he is the co-inventor of 03 molecules which are in clinical development. He has 10 patents and over 20 publications in various international journals. Additionally, he is the co-author of 01 book in bioinformatics and 02 book chapters. He is also the member of special committee of Jawaharlal Nehru University, New Delhi. He had set up the state-of-the-art informatics laboratories in various pharmaceutical companies like Jubilant Biosys, Dr. Reddys's Laboratories, Lupin ltd. Presently he is heading the CADD division in Aragen Lifesciences Hyderabad and is responsible for digital transformation and development of various proprietary platform technology using AI/ML tools to aid drug discovery and development.

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Towards a Digital wave in Drug Discovery and Development-Pharma4.0

Abstract

Tufts Center for the Study of Drug Development (CSDD) states that the cost of developing a new prescription drug is approximately $2.6 billion-which is 145% increase, comparing to the cost over a decade-with a timeline of over 10-15yrs. With rising cost coupled with lesser opportunity for low hanging fruits in drug discovery and development, pharmaceutical industry is in a terminal decline phase, and the returns on investment on new drugs that do get to market is not aligning with the massive investments that pharmaceutical companies put into R&D.

The R&D phase of developing a new pharmaceutical product or drug is very long and expensive in comparison with conventional products, so using Industry 4.0-related technologies in the drug development process might bring enormous benefits to the biomedical and pharmaceutical industries.

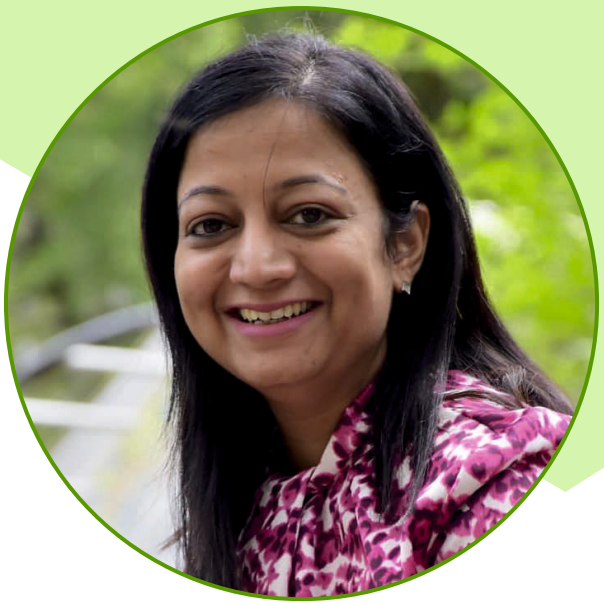
Digital efforts like automation, AI/ML and Blockchain based technologies are not the luxury but a necessity which any health care organization cannot afford not to have. With petabytes of data lying in the pharmaceutical companies' databases from both preclinical and clinical data, it has become a imperative to investigate the datasets with a newer perspective and with focused lenses. The integration of big data and genomics is an important trend in the use of AI in drug discovery. By integrating genomics data with AI, researchers can identify specific genetic variations that are associated with certain diseases, which can lead to the development of personalized therapies.

Quince Market Insights forecasted that the global AI/ML in the Drug Discovery market is to grow at a CAGR of 28.34% during the period 2023 to 2032. Furthermore, the increasing use of big data analytics and the growing use of virtual screening in drug discovery are also expected to contribute to the market growth.

In this perspective the present talk would canter towards adoption of newer technology platforms to accelerate the drug discovery and development. Technology like automation, implementation of HPCs, and advanced algorithms for drug discovery would be covered.

Dr. Deeksha Bhartiya

Founder & Director
Genomiki, Ghaziabad, Uttar Pradesh



Profile

Dr. Deeksha Bhartiya is a leading bioinformatics scientist, the founder and director of Genomiki Solutions, a startup specialising in providing genome-informatics solutions. With a Ph.D. from the CSIR-Institute of Genomics and Integrative Biology and postdoctoral experience at Karolinska Institutet in Stockholm, she possesses over a decade of computational genomics expertise. Her leadership has propelled Genomiki Solutions to gain incubation support from prestigious centres such as NSRCEL at IIM Bangalore and IIT Kanpur among others. Known for her robust computational and programming skills, coupled with extensive experience in high-throughput biological data analysis, Dr. Bhartiya is a leading figure in the genomics field. Her regular presentations at national and international conferences demonstrate her significant contributions to genomics research and clinical applications, driving innovation in healthcare diagnostics through Genomiki's advanced genome-informatics and bioinformatics solutions.

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Empowering Medical Insights with Genome Informatics

Abstract

Genomics is revolutionising modern medicine, providing critical insights for more accurate diagnoses, personalised treatments, and better patient outcomes. Genome-informatics leverages advanced computational techniques to interpret genetic data and empowers healthcare professionals to make more informed decisions. Through this talk, we'll explore the breakthroughs in understanding genetic mutations, the role of big data in predicting disease risks, and the evolution of precision medicine. By harnessing the power of genomics, we are transforming healthcare into a more proactive and preventative practice through our germline and somatic genomics solutions. These solutions pinpoint the causative variants and help the doctors take an accurate and precise decision using personalised reports and recommendations.

Session: Partners & Collaborators

Prof. M. S. Madhusudan

Prof. Arnab Mukherjee

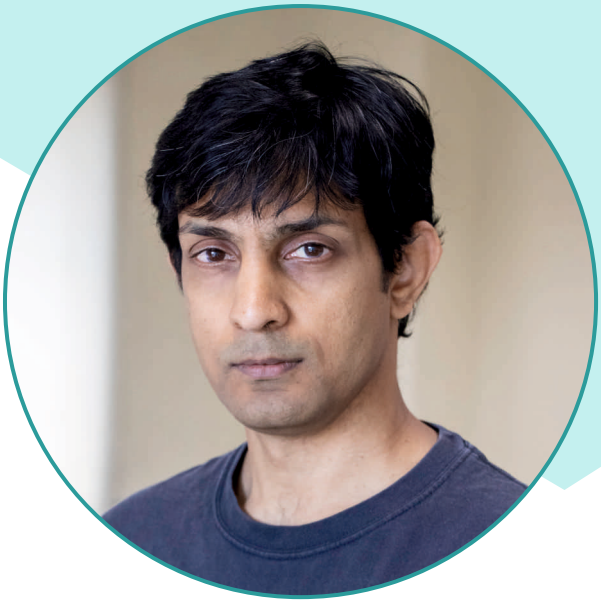
Dr. Durba Sengupta

Dr. Dharani Gopal

Dr. Govardhan Reddy

Prof. M. S. Madhusudan

Professor, Indian Institute of Science Education and Research (IISER), Pune



Reading genomes

Absrtact

Interacting proteins usually bind 5-6 base pairs of DNA. We looked at distributions of 5/6-mer DNA motifs, in whole chromosomes and in smaller sections, across the whole genome to get insights into how proteins read genomic sequences. The distribution of motifs in the genome is non-random as established by their observed to expected (OE) ratios at all examined length scales. We correlated the motif distributions in promoter regions of genes to one another and found evidence for translocations, gene regulatory networks and even data pertaining to spatial proximity of regions between genes. In general, correlating genomic regions by motif distribution comparisons alone is rife with functional information.

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Prof. Arnab Mukherjee

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Reinforcement Learning Helix Disrupting Mutation

Absrtact

Helices are one of the most important secondary structural motifs within proteins. Often helix to random coil or helix to beta sheet transition leads to disruption of the protein and its function leading to numerous diseases. Although amino acids are categorized based on helix propensity scales that provide an idea about such helix disrupting mutations, the protein environment around the helix also dictates the stability of the helix. For a protein with n amino acids, there are (_^n)C_k × 〖19〗 ^k possible k-point mutations possible. However, such a large number of trials are not practically feasible. Here, we employ reinforcement learning along with the state-of-the-art machine-learned protein structure prediction to tackle this challenge and develop a predictive model for helix-disrupting mutations. We start with a toy model consisting of helices with only 30 amino acids and train different models. Our results show that our model is successful in disrupting helical structures. We expand our methodology to effectively disrupt helices in proteins and confirm these outcomes through all-atom explicit water free energy calculations using well-tempered metadynamics. The results from our investigations serves as a proof-of-concept for developing similar models, showcasing the potential of reinforcement learning to tackle issues related to protein structure disruption.

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Dr. Dharani Gopal

Scientist G & Group Head, Marine Biotechnology Division, National Institute of Ocean Technology (NIOT), Chennai

Profile

Dr. Dharani Gopal is a distinguished Scientist G and Group Head at the Marine Biotechnology Group, National Institute of Ocean Technology, Chennai. Specializing in Plankton Ecology & Biology and Marine Biotechnology, Dharani holds M.Sc., M.Phil., and Ph.D. As an accomplished researcher, Dr. Dharani has an impressive record of patents (9) and publications, including 122 journal articles and 21 book chapters. Dharani's expertise extends to Open Water SCUBA Diving and EFR Instructor, certified by PADI. Dr. Dharani has made significant contributions, including the development of a microalgal harvesting system, processes for extracting pharmacoactive nutrients from marine algae, and the production of lutein. Dharani's work also involves biotechnological solutions like detecting virulent genes of Enterococcus faecalis, compositions for bioremediation of oil spills, and recombinant technologies for cosmeceutical and chemotherapy applications. Dharani's excellence in ocean sciences has been recognized with several awards, including the Young Scientist Award by the Ministry of Earth Sciences, Government of India in 2010, and Best Paper Awards at national and international conferences in 2008 and 2006. Additionally, Dharani is an active member of several committees and professional bodies, including the Commission for the Conservation of Antarctic Marine Living Resources (CCAMLR), the Coastal Aquaculture Authority, and various technical advisory committees related to biotechnology and seaweed farming.

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Marine Genomics and High-Performance Computing: The Indispensable Alliance

R. Vijaya Raghavan*, T. J. Sushmitha, and G. Dharani*
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Abstract

Deep-sea environments, with their extreme conditions such as high pressure, low temperature and absence of sunlight, harbor vast and unique microbial communities. These microbes play vital roles in global biogeochemical cycles and hold untapped potential for biotechnological and pharmaceutical innovations. Marine bioresources have always been considered as sources of novel biomolecules with potential applications in the field of biotechnology and industries. The vast diversity of marine microbes, from bacteria to archaea and viruses, remains largely unexplored due to the inherent challenges in accessing and analyzing their genomic data. As of 2024, there are several petabytes of sequencing data from marine microbial genomes publicly available, with additional data continually generated by international research efforts. Advances in high-throughput sequencing technologies have led to a surge in microbial genome data, providing insights into the metabolic pathways, adaptation mechanisms, and ecological roles of these organisms. However, the scale and complexity of these datasets require the integration of high-performance computing (HPC) to efficiently process, store, and analyze large volumes of genomic data. HPC enables the application of sophisticated algorithms for genome assembly, annotation, and comparative genomics, as well as modeling microbial interactions and simulating oceanic processes. With exascale computing, massive amounts of sequencing data from continuous oceanic samplings can be processed, analyzed, and correlated with environmental parameters (e.g., temperature, salinity, pH) to detect trends or sudden changes in microbial ecosystems. The parallel computing capabilities of exascale systems also allow simulations of microbial interactions across vast, spatially-expansive marine environments, accounting for thousands of species and their dynamic behaviors, all at high resolution. The immense processing power of exascale computing allows for the application of deep learning and other AI techniques to analyze and classify vast amounts of genomic data, enabling the discovery of new microbial species and helping track microbial evolution at an unprecedented scale. By combining marine microbial genomics with exascale computing, researchers can significantly enhance their ability to explore the vast and complex world of marine microbes. This integration will not only deepen our understanding of oceanic ecosystems but also drive innovations in fields such as environmental monitoring, bioremediation, and climate change mitigation.

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Dr. Durba Sengupta

Principle Scientist and Associate Professor (AcSIR)

Signatures of GPCR-lipid Interactions: Specificity, Synergy and Energetics

Absrtact

The G protein-coupled receptors (GPCRs) are membrane receptors that play a central role in cell signaling and pharmacology. The interaction of lipids with GPCRs has been shown to modulate and dictate several aspects of GPCR organization and function. In this talk, I will discuss the diversity of lipid interaction sites that have been identified from molecular dynamics studies and compare to structural data. Using coarse-grain simulations, we identified several GPCR-lipid, in particular GPCR-cholesterol signatures and highlight the common and specific features. Further, using a set of similarity coefficients, we classify lipids that bind at the receptor together as synergistic co-binding, and those that bind individually as competitive. Not surprisingly, the ganglioside GM1 and cholesterol show a synergistic co-binding. In contrast, certain lipid pairs such as cholesterol and sphingomyelin appear to be in competition at several sites, despite their co-existence in lipid nanodomains. To quantify these interactions, we estimate the energetics and dynamics of lipid association. We show that lipids bind to the receptor with varying energetics of 1-4 kT, and timescales of 1-10 μs. Multi-exponential fitting of the contact probability suggests a three-step model, that we correlate with the annular, intermediate and non-annular sites. High barrier heights are estimated between the states that reduce the association/dissociation kinetics. The results highlight that GPCR-lipid interactions are driven by both thermodynamic interactions and the dynamical features of lipid binding.

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Dr. Govardhan Reddy

Associate Professor, Indian Institute of Science (IISc), Bengaluru

Profile

Dr. Govardhan Reddy is an associate professor at the Solid State and Structural Chemistry Unit, Indian Institute of Science (IISc), Bengaluru. His current research interests are in theoretical/computational biophysical chemistry and biophysics, focussing on structural transitions in biomolecules.

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Salt Induced Transitions in the Conformational Ensembles of Intrinsically Disordered Proteins

Abstract

Salts and pH modulate the behaviour of intrinsically disordered proteins (IDPs) and influence the formation of membraneless organelles through liquid–liquid phase separation (LLPS). In low ionic strength solutions, IDP conformations are perturbed by the screening of electrostatic interactions, independent of the salt identity. In this regime, insight into the IDP behaviour can be obtained using the theory for salt-induced transitions in charged polymers. However, salt-specific interactions with the charged and uncharged residues, known as the Hofmeister effect, influence IDP behaviour in high ionic strength solutions. There is a lack of reliable theoretical and computational models in high salt concentration regimes to predict the salt effect on IDPs. We propose a simulation methodology using a coarse-grained IDP model and experimentally measured water-to-salt solution transfer-free energies of various chemical groups to study the salt-specific transitions induced in the IDPs conformational ensemble. We probed the effect of three different monovalent salts on five IDPs belonging to various polymer classes based on charged residue content. We demonstrate that all the IDPs belonging to different polymer classes behave as self-avoiding walks (SAWs) at physiological salt concentration. In high salt concentrations, the transitions observed in the IDP conformational ensembles depend on the salt used and the IDP sequence and composition. An important implication of these results is that a suitable salt can be identified to induce IDP condensation through LLPS.

Poster Abstracts

SB: Structural Biology

CG: Computational Genomics

AS: Algorithms and Software

GS: General Science

SB1: Design Synthesis and Biological Evaluation of ABCB1 Inhibitors

Sinhgad College of Pharmacy, Vadgaon BK., Pune
Rupali Barhate and Rajesh Patil

Abstract

The recurrence of cancer and patient mortality are often associated with chemotherapy induced drug resistance. The ATP binding cassette subfamily B member 1 ABCB1 transporter is overexpressed in tumors, contributing to this resistance. However, most ABCB1 inhibitors have been ineffective in clinical trials. In this study, we propose a novel approach to developing ABCB1 inhibitors. The ZINC database, which contains millions of small molecules, was screened, and 641 compounds with structural and shape similarity to Zosuquidar were identified using Lipinskis rule and shape similarity criteria. These compounds were selected for multiple ligand simultaneous docking, which provided the means of simultaneously dock two zinc compounds at the drug binging site and at the adjacent access tunnel. A molecular docking study provided insights into the interactions between the compounds and the target protein. The docking process yielded several compounds with higher binding energies. Ultimately, 82 hits with higher binding energies than Zosuquidar were selected. Subsequently, using the Langevian Rotametically Induced Perturbation (LRIP) method (a non equilibrium MD approach aimed at identifying slow conformational changes in a binding site) the conformations of ABCB1 varying in the binding site residues were generated and used in ensemble docking of 82 hits on 23 rotamers of ABCB1. The reranking of docked hits identified top 20 hits having lower and better binding free energies than the Zosuquidar. The Molecular dynamics simulations on the resulting complexes are in progress.
Binding site residues were generated and used in ensemble docking of 82 hits on 23 rotamers of ABCB1. The reranking of docked hits identified top 20 hits having lower and better binding free energies than the Zosuquidar. The Molecular dynamics simulations on the resulting complexes are in progress.

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SB2: Exploration of phytochemical compounds from Millets as NRF2 activators using molecular docking and molecular dynamics simulation approaches

Nalban Nasiruddin, Manish wanjari, Sudhir Matte, Anurag kumar, Munaf Tamboli, Pallavi jamadagni, Arun Manohar and Gurav
CCRAS Regional Ayurveda Research Institute, Pune

Abstract

Oxidative stress plays vital role in progression of several diseases like cardiovascular, neurological and gastrointestinal disorders. On regular consumption millets are known to have beneficial effects. They are also rich in phytochemicals. In the current study these phytochemicals are aimed against the complex of KEAP1-NRF2 and activating NRF-2. NRF2 is a potent inducer of anti-oxidant enzymes like heme-oxygenase and superoxide dismutase. Molecular docking was conducted to study compounds that can form an interaction similar to 1VX (co-crystalized ligand). CDOCKER interaction energies of isovitexin, vitexin, kaempferol, protocatechuic acid, and vanillic acid were better than 1VX. The best three molecules (isovitexin , vitexin, kaempferol) based on CDOCKER interaction energy were subjected to molecular dynamic simulation for 100ns which revealed their stability at active site. Further MM-PBSA binding free energy of phytochemicals were calculated. Values of isovitexin, vitexin, Kaempferol and 1VX are -32.0468kcal/mol, -24.8182 kcal/mol -4.1739 Kcal/mol, and -10.2521 Kcal/mol, respectively, which indicate high degree of binding compared to co-crystallized ligand IVX. Results indicated that selected compounds (isovitexin, vitexin, kaempferol) can act as NRF2 activators which further can be conformed through in vitro and in vivo studies.

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SB3: Structure and ligand-based design, synthesis and biological evaluation of dual inhibitors of select kinase targets

Suvarna Vakare and Rajesh Patil
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Abstract

CDK4/6 and FLT3 are key targets in cancer therapy due to their involvement in cell cycle progression and survival pathways. This study aimed to develop a 2D Quantitative Structure Activity Relationship (QSAR) model to predict dual inhibitory activity against both CDK4/6 and FLT3 and to identify the potential hits from the ZINC database through shape based virtual screening. A dataset of chemical compounds with known affinity for these targets was prepared by using literature review. Using a genetic algorithm-multiple linear regression (GA-MLR) approach and PaDEL descriptors, predictive models for CDK4/6 and FLT3 inhibitors were constructed. The models were validated internally and externally, showing predictive accuracy with RÂ² = 0.8152, QÂ²_loo = 0.7136, and R2ext: 0.7360 for CDK4/6, and RÂ² = 0.8388, QÂ²_loo = 0.7175, and R2ext: 0.7366 for FLT3. A potent dual CDK4/6 and FLT3 inhibitor (compound 23K) was used as a reference to conduct a virtual screening of the Zinc database based on shape similarity. Further, the screened compounds were filtered using a modified version of Lipinskiâ€™s rule of five, reflecting the physicochemical properties of compound 23K. The developed QSAR models were then applied to predict the inhibitory activity of the filtered compounds against both CDK4/6 and FLT3. Currently, the identified hits are being investigated through the molecular docking and molecular dynamics studies. This study demonstrates the successful application of QSAR modelling and virtual screening to identify new lead compounds targeting both CDK4/6 and FLT3, potentially offering improved therapeutic options in cancer treatment.

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SB4: Free energy estimation using Binding Free Energy EstimatorR

Rohan J Meshram, Gor Mihir Deepakbhai
Bioinformatics Centre, SPPU, Pune

Abstract

The accurate estimation of free energy is crucial for understanding molecular processes in various fields, including drug discovery and materials science. This work introduces BFEER, a novel computational tool designed to efficiently calculate free energy differences using the Molecular Mechanics Poisson-Boltzmann Surface Area (MMBPSA) and Linear Interaction Energy (LIE) methods. BFEER provides a user-friendly interface for input preparation and result analysis, making it accessible to researchers with diverse computational backgrounds. By offering a robust and efficient platform for free energy estimation, BFEER aims to contribute to the advancement of computational chemistry and facilitate the study of complex molecular systems.

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SB5: 3D Structure-Based Functional Annotation of Hypothetical Proteins in Escherichia coli and Mycobacterium tuberculosis

Sejal Agarwal, Dr. Shekhar C. Mande, Dr. Payel GhoshBioinformatics Centre, SPPU, Pune

Abstract

Hypothetical proteins constitute a substantial proportion of bacterial genomes, yet remain functionally uncharacterized due to limited sequence homology with annotated proteins. Elucidating the functions of these genomic hypotheticals is crucial for comprehensively understanding bacterial physiology, pathogenesis, and molecular mechanisms, particularly in model organisms such as Escherichia Coli and Mycobacterium tuberculosis. In this investigation, we employed a comprehensive multi-tiered approach to annotate the potential functions of hypothetical proteins. Initial sequence-based homology searches using Basic Local Alignment Search Tool for proteins (BLASTp) revealed that approximately 80% of the hypothetical proteins demonstrated significant sequence similarity to known proteins, facilitating preliminary functional annotations. The remaining 20% of proteins, lacking significant sequence homology, were subsequently subjected to advanced three-dimensional structural prediction utilizing AlphaFold2. Structural analyses were conducted through systematic comparisons with well-curated protein structural repositories, including the Protein Data Bank (PDB) and Structural Classification of Proteins (SCOP) database. Comparative structural alignments and fold recognition algorithms were applied to infer potential functional domains and molecular interactions for the proteins without clear sequence-based annotations. The proteins without sequence homology exhibited diverse structural characteristics, with some revealing novel structural motifs suggesting potentially unique molecular functionalities. These findings highlight the complementary nature of sequence-based and structure-based computational approaches in protein functional annotation. Our methodology demonstrates a robust framework for addressing the persistent challenge of characterizing hypothetical proteins, bridging computational prediction with potential experimental validation in microbial genomic research. The approach provides a comprehensive strategy for expanding our understanding of uncharacterized protein functions, particularly in bacterial systems.

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SB6: Computational Analysis of Biofilm Components and Antibiotic Synergy to Combat Hospital-Acquired Infections

Mansi Kumari, Madhu Choubey Anup Kale
MIT-WPU Pune, Kothrud, Pune

Abstract

The increasing threat of antimicrobial resistance (AMR) in opportunistic pathogens constitutes a significant global health crisis. According to the projections from the Indian Council of Medical Research (ICMR) estimating 10 million deaths annually by 2050 if not addressed. Opportunistic pathogens that form biofilms contribute to persistent infections, especially in immunocompromised individuals, including those with cystic fibrosis, burns, or chronic wounds. Biofilm formation markedly increases resistance, resulting in antibiotic tolerance that can reach up to 1,000-fold.

This research implements In silico molecular docking and dynamics simulations to investigate interactions between biofilm matrix components and pharmaceutical agents. The experiment includes standard antibiotics—ceftazidime (targeting key biofilm forming exopolysaccharides Psl [polysaccharide synthesis locus] and Pel [pellicle matrix component]), clarithromycin (targeting alginate, a biofilm constituent), and the phytochemical lutein from calendula, which affects the quorum-sensing molecule Rhl(regulation of rhamnolipid biosynthesis). The findings demonstrate that ceftazidime exhibits stronger binding with Psl (-138.097 kcal/mol) and Alg (-139.743 kcal/mol) compared to clarithromycin with Psl (-14.72 kcal/mol) and Alg (-78.2688 kcal/mol), while lutein shows a binding energy of -59.8413 kcal/mol with Rhl. Molecular dynamics simulations evaluated the stability of ligand-protein interactions through analyses of natural charge, electrostatic potential, and frontier molecular orbitals. This methodology emphasises the significance of computational models in healthcare, facilitating drug repurposing and the integration of traditional medicine to address antimicrobial resistance (AMR) and enhance healthcare resilience.

Keywords: Antimicrobial resistance, Molecular docking, Drug repurposing, Calendula, Rhamnolipid, Polysaccharide synthesis locus (Psl), Pellicle matrix component (Pel).

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SB7: Exploring Plant Derived Acetylcholinesterase Inhibitors as Therapeutic Candidates for Alzheimers Disease

Devaki Sethi, Hari Krishna Thene, Pavan K Madasu, Onkara Perumal P and Thyageshwar Chandran
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Abstract

Alzheimerâ€™s disease (AD), a serious neurodegenerative disorder affecting memory and cognition in the elderly, is linked to declining cholinergic neurons, which produce the neurotransmitter acetylcholine (ACh). Acetylcholinesterase (AChE) breaks down acetylcholine in the synaptic cleft, and has become a primary focus in AD drug discovery. Inhibiting AChE extends the presence of acetylcholine in synaptic junctions, thereby enhancing cholinergic neurotransmission and mitigating cognitive symptoms. We have prepared a library of compounds with neuroprotective functions and have screened for their AchE inhibitory activity. Our work resulted in the identification of 56 bioactive compounds. Of these, 23 compounds have passed the ADMET analysis and were studied for their inhibitory activity by employing molecular docking. N-trans feruloyltyramine and O-methylnorbelladine showed strong binding affinities with CDOCKER energies of -37.7537 and -34.7304 respectively. These findings suggest that these compounds could serve as promising candidates for further development as novel therapeutic agents targeting Alzheimerâ€™s disease. The insights gained from this research pave the way for future investigations aimed at discovering and optimizing new drug candidates to alleviate the cognitive decline associated with AD.

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SB8: Decoding G Protein Selectivity in the Beta-1 Adrenergic Receptor Using Machine Learning: Uncovering Coupling Signatures

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Abstract

G protein-coupled receptors (GPCRs) play an instrumental role in cell signaling for the regulation of a variety of cellular responses. The intracellular binding proteins, the G proteins mediate transduction processes by coupling to GPCRs, but the mechanism of selective coupling of different G protein subtypes to a given GPCR is not well characterized. To address the question of G protein selectivity in the Î²1-adrenergic receptor, we have coupled molecular dynamics simulations with machine learning approaches to identify structural and dynamic features of these protein complexes. Atomistic molecular dynamics simulations of the Î²1-adrenergic receptor in complex with a cognate (GÎ±s), a non-cognate (GÎ±i/o) and a promiscuous (GÎ±q11) subunit of G proteins were performed. A machine learning classifier was trained on the simulation data to predict the important structural determinants responsible for coupling in each G protein. Using this model, we show that the coupled dynamics of transmembrane helix 5 and 6 are important predictors of G-protein specificity. Further, we show that the apo-receptor complexes are much more dynamic and do not retain the signatures of the G protein specificity. Our results indicate that machine learning approaches could be important to identify patterns in complex molecular dynamics simulations and for better characterization of highly plastic receptor-protein interactions. Our work is an important step to identify factors conferring G-protein specificity in the Î²1-adrenergic receptor.

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SB9: In Silico Design and Screening of Aptamers for Myoglobin and Troponin in Predictive Mapping of Cardiovascular Disease

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Abstract

Cardiovascular diseases (CVDs) are the leading cause of mortality worldwide, responsible for over 20.5 million deaths annually, with 85% resulting from heart attacks and strokes. Current diagnostic approaches often lack the sensitivity required to detect CVDs in early stages, underscoring the need for predictive mapping methods that can identify cardiovascular risks at onset, thereby reducing mortality rates. Biomarkers such as Troponin and Myoglobin are highly valuable in this context due to their specificity and sensitivity in signalling cardiac events. Troponin I exhibit nearly 100% specificity for cardiac muscle injury, while Myoglobin provides 70-80% sensitivity within the first 1-3 hours post-onset, offering complementary, rapid-response diagnostic capabilities.

This project focuses on the in-silico design and screening of aptamers for Myoglobin and Troponin to enhance early diagnostic precision. A total of 10 Myoglobin and 32 Troponin sequences were evaluated through molecular docking and molecular dynamics simulations. Key interaction parameters—including hydrogen bond formation, contact surface area, binding free energy, interaction energy, Root Mean Square Deviation (RMSD), and Root Mean Square Fluctuation (RMSF)—were assessed to identify aptamers with the strongest, most stable affinity for these targets. This approach not only supports early CVD detection but also bypasses the conventional SELEX (Systematic Evolution of Ligands by Exponential Enrichment) process, streamlining high-affinity aptamer development. These findings underscore aptamers' potential as precise, reliable tools for CVD predictive mapping, contributing to reduced CVD-related mortality.

Keywords:
Cardiovascular diseases, aptamers, predictive mapping, molecular docking, molecular dynamics simulations, biomarkers, Myoglobin, Troponin, SELEX-free development.

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SB10: Insights into antineoplastic properties of Tinospora cordifolia using network pharmacology and molecular docking

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Abstract

Tinospora cordifolia, also known as Guduchi or Amrita, is a climbing shrub found throughout tropical regions of South Asia. This plant is widely utilized in Ayurvedic medicine for treating various disorders, including neoplastic growths. A thorough literature review was carried out to identify bioactive compounds in Tinospora sp., and their corresponding gene targets were determined using the ChemBL database or predicted through BindingDB and SwissTargetPrediction. DisGeNet database was used to enrich 79 out of 116 gene targets based on their documented involvement in cancer-related pathways in humans. A STRING analysis was performed to identify hub genes, with pathways assigned using KEGG mapper. Cytoscape analysis was used to create a comprehensive pharmacological network and to highlight multi target - multi ligand interactions. To confirm binding, the 15 main hub genes were docked with their respective ligands (bioactives) using PyRx. Several bioactive compounds in Tinospora cordifolia were found to influence multiple known cancer-related pathway genes, such as AKT2, HRAS, KRAS, IGF1R, SRC, and STAT3. Moreover, unique bioactive compounds in the plant, including Tinocordiside and Cordifolioside, showed effective binding to targets like HRAS and KRAS. This study highlights Tinospora cordifolia's potential to modulate multiple cancer-associated pathways.

Keywords: Tinospora cordifolia, Guduchi, Amrita, network pharmacology, molecular docking, Ayurveda, BindingDB, SwissTargetPrediction, DisGeNet, STRING, KEGG Mapper, Cytoscape, PyRx, ligand, bioactive, AKT2, HRAS, KRAS, IGF1R, SRC, STAT3, Tinocordiside, Cordifolioside, cancer, pathway, neoplasm.

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SB11: Inhibition of β-Lactoglobulin Fibrillation through the Application of 2D Material

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Abstract

Understanding the morphological and structural features of misfolded proteins is a hot topic in current research. Amyloid plaque deposition in the brain, kidneys, liver, heart, and pancreas is associated with diseases such as Alzheimer's, Parkinson's, prion diseases, Huntington's, and type-2 diabetes. The exact mechanisms of fibrillation and defibrillation remain unclear. This study primarily focuses on the mechanism of defibrillation of β-Lactoglobulin (β-Lg) protein using 2D Graphene Oxide (GO). GO is a sheet-like structure that can disrupt the rod-like fibril structure of a protein, reversing it back to the dimeric structure of the protein in neutral pH. This phenomenon is elucidated using spectroscopy, microscopy, and Small-Angle X-ray Scattering (SAXS) techniques. The inhibitory effect of GO on the aggregation of β-Lg is indicated by the Thioflavin (ThT) assay. The ThT results show that GO can inhibit the aggregation pathways of the protein. The secondary structure alterations of the protein were recorded by using circular dichroism. From the SAXS study, the pair distribution function p(r) plot suggests that the dimeric native structure of β-Lg protein changes to a possibly elongated shape. In the presence of GO, the dimeric structure is restored. Scanning Electron Microscope (SEM) images show that the rod-like fibril structure of β-Lg disappears with the penetration of the GO sheet. The effect of GO on β-Lg aggregation provides significant insights into the inhibitory effects of 2D materials on protein fibrillation, opening a new avenue for therapeutic approaches against neurodegenerative diseases and other amyloid plaque-related disorders.

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SB12: Structure-Based Pharmacophore Feature Extraction for the Discovery of Potent SARS-CoV-2 Main Protease Inhibitors

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Abstract

The ongoing threat of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) necessitates continued development of effective antiviral therapies. Targeting the SARS-CoV-2 main protease (Mpro) remains a promising long-term strategy. In this study, we adopted a structure-based drug design approach that integrated pharmacophore modeling, virtual screening, molecular docking, and molecular dynamics (MD) simulations to identify novel potent Mpro inhibitors. A five-point pharmacophore model (AADHH), derived from known Mpro inhibitors with IC50 values ranging from 0.013 to 34 nM, was used to screen the DrugBank (DB) and Natural Product Atlas (NPA) databases using Schrodinger PHASE. GLIDE extra precision (XP) docking was further used to identify top hits. The best ten compounds were selected for analysis, including Absorption, Distribution, Metabolism, and Excretion (ADME) property prediction using QikProp. The virtual screening of the databases yielded 2564 hits from DB and 1822 hits from NPA, with 84% actives based on Receiver Operating Characteristic curve (ROC) evaluation. Eight compounds from DB and three from NPA showed XP scores greater than the binding affinity of a control inhibitor Nirmatrelvir. In 100 ns MD simulations, DB11879 (XP score = -9.075 kcal/mol) and NPA008908 (XP score = -8.962 kcal/mol), demonstrated greater stability (RMSD = 2.2 Å and 1.9 Å respectively) than Nirmatrelvir (XP score = -7.549 kcal/mol; RMSD = 3.1 Å). Both compounds formed strong hydrogen bonds with the Mpro catalytic dyad Cys145 and the conserved residue Glu166. The findings suggest DB11879 and NPA008908 as promising lead compounds against SARS-CoV-2, warranting further in vitro and in vivo evaluation.

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SB13: Molecular Insights into Indole-carbinol Hybrids: Targeting BCL-2 for Anti-Cancer Drug Development through Docking and Molecular Dynamics Simulation

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Abstract

Protein-ligand interaction studies are fundamental for understanding the mechanisms of biological processes at the molecular level. The structures of protein-ligand complexes propose a theoretical basis for the design and discovery of new drug targets. Indole based compounds are well-known for their diverse biological studies, including anti-cancer studies as well. In the present study, three indole-carbinol hybrids (IC-1, IC-2 and IC-3) were investigated for their interaction with a targeted protein. All the three compounds had previously shown to exhibit promising activity against MCF-7 breast cancer cell line. Literature review analysis identified BCL-2, an anti-apoptotic protein, as a potential target for indole-carbinol related compounds. The ADMET properties of all the three hybrids were evaluated to ensure their drug likeliness and were docked against BCL-2 protein using AutoDock Vina to ascertain their molecular interactions. The finest conformations of each docking algorithm were subjected to molecular dynamic simulations to analyze RMSD, RMSF, Rg, SASA and hydrogen bonding at the protein-ligand interface. Compound IC-3 in particular displayed the highest stability, maintaining consistent interactions with the protein throughout the simulation, projecting it as a highly promising candidate for further molecular exploration.

Keywords: Docking, Anti-apoptotic protein, Hydrogen bonding, Conformations, Drug likeliness.

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SB14: Exploring Purine Analogues as Inhibitors against Katanin, a Microtubule Severing Enzyme using Molecular Modeling Approach

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Abstract

Katanin, a key protein in cellular architecture, plays a crucial role in severing microtubules, which are vital cytoskeleton components. Given its central involvement in cell division and proliferation, katanin represents a promising target for therapeutic intervention, particularly in cancer treatment. Inhibiting katanin's function could potentially hinder the uncontrolled growth of cancerous cells, making it an attractive target for novel anti-cancer therapies. Previous studies have shown that purine-based compounds exhibit a strong affinity for microtubule-severing enzymes. In this study, we aim to identify potential purine-type inhibitors of katanin using molecular modeling techniques. A total of 276,280 purine-type compounds from the PubChem database were subjected to structure-based high-throughput virtual screening, followed by ADME prediction, PASS analysis, and molecular docking studies. These efforts led to the identification of two potent compounds: PubChem CID 122589735 and 123629569, which demonstrated strong binding interactions with katanin. Molecular dynamics simulations further revealed that these compounds effectively altered katanin's conformation when compared to ATP. Additionally, binding energy calculations indicated that PubChem CID 122589735 exhibited the strongest binding affinity for katanin, with the binding free energy ranking as follows: 122589735 > 123629569 > ATP. Our findings suggest that the screened compounds, particularly PubChem CID 122589735, hold promise as potential katanin inhibitors. These compounds could play a significant role in the development of new anti-cancer therapies targeting a variety of carcinomas. Future research, including in vitro and in vivo studies, is essential to assess the efficacy and safety of these inhibitors, paving the way for innovative cancer treatments.
Keywords: Katanin, Microtubule, Purine analogues, structure-based drug design, Molecular dynamic simulations

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SB15: Assessment of Sedative - Hypnotic Activity of Benzyl Benzoate using Integrated Computational Pharmacology and Mammalian Model

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Abstract

Increase in clinical use of the currently marketed and synthetic sedative-hypnotics is associated with number of issues including adverse effects, drug abuse, withdrawal syndromes and severe toxicities. The aim of the current study was to investigate the phytoconstituents to identify a sedative-hypnotic with good efficacy and lesser side effects based on their binding affinities towards GABAA receptor and predicted physicochemical and pharmacokinetic properties.

In present study we screened 42 phytoconstituents for GABAA receptor binding site. Natural compounds, like Benzyl Benzoate present as one of the major constituents of fragrant flowers like Jasmine was selected based on binding affinity to screen for sedative-hypnotic effects. The sedative activity of Benzyl Benzoate was screened by testing the locomotor activity using an actophotometer and hole-board test for assessing the explorative behavior and curiosity. The hypnotic effects were studied using thiopentone sodium induced sleeping time test. Benzyl benzoate showed significant sedative effects by decreasing locomotor activity as well as explorative behavior in mice, when compared with the pretreatment reading of each group. Decrease in onset and increase in duration of sleep of thiopentone-induced sleep in mice, which demonstrated its hypnotic effects as compared to the control group. Binding of Benzyl Benzoate to benzodiazepine site was ensured by using selective antagonist Flumazenil. Flumazenil significantly replaced benzyl benzoate from its receptor as a result we found awakening behavior pattern in mice.

Thus, in the present study, Benzyl Benzoate has shown to possess significant sedative as well as hypnotic properties mediated via binding with GABAA receptor.

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SB16: Molecular Docking and Pharmacodynamic Analysis of Quercus infectoria and Ficus benghalensis Against Streptococcus mutans

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Abstract

Dental biofilms, commonly referred to as dental plaque, develop in the oral cavity through the adhesion of microorganisms to one another or the surface of teeth. Biofilm protects the micro-organism from mechanical stress and antimicrobial agents thus, oral bacterial biofilms are a primary driver of antibiotic resistance and contribute significantly to the development of severe periodontal infections. Streptococcus mutans is primarily associated with dental biofilms, with glucan-binding protein (GbpC) playing a key role in biofilm formation. The role of GbpC in biofilm formation and adhesion is fundamental, making it a major contributor to the cariogenic properties of S. mutans. This study explores a computational approach to predict the binding interactions between phytochemical extracts of Quercus infectoria (Gall) and Ficus benghalensis (Bark) with the GbpC protein, aiming to inhibit the adhesion of S. mutans to tooth surfaces. The study employs AutoDock for molecular docking analysis. Additionally, pharmacodynamic studies were conducted using SwissADME, ADMET 3.0, and Molinspiration to evaluate physicochemical properties, and toxicity predictions, respectively. Docking results revealed the binding affinities of ligands from Quercus infectoria (Gall) as follows: syringic acid (-5.5 kcal/mol), flavylium (-7.0 kcal/mol), ellagic acid (-5.3 kcal/mol), and gallic acid (-7.4 kcal/mol) and for Ficus benghalensis (Bark), the binding affinities were: leucopelargonidin (-8.0 kcal/mol), and tiglic acid (-4.5 kcal/mol). Docking scores indicated that all six selected ligands have potential as GbpC inhibitors. Among the ligands, the binding affinities of flavylium, gallic acid, and leucopelargonidin indicate stronger interactions with the target protein, suggesting greater potential for drug efficacy.

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SB17: Ligand and structure-based computational designing of multi-target molecules directing FFAR-1, FFAR-4 and PPAR-G as modulators of insulin receptor activity

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Abstract

Multi-agent therapies are an important treatment modality in many diseases based on the assumption that combining agents may result in increased therapeutic benefit by overcoming the mechanism of resistance and providing superior efficiency. Extensively validated 3D pharmacophore models for free fatty acid receptor-1 (FFAR-1), free fatty acid receptor-4 (FFAR-4), and peroxisome proliferator-activated receptor-G (PPAR-G) was developed. The pharmacophore model for FFAR-1 (r2 = 0.98, q2 = 0.90) and PPAR-G (r2 = 0.89, q2 = 0.88) suggested that one hydrogen bond acceptor, one hydrogen bond donor, three aromatic rings, and two hydrophobic groups arranged in 3D space are essential for the binding affinity of FFAR-1 and PPAR-G inhibitors. Similarly, the pharmacophore model for FFAR-4 (r2 = 0.92, q2 = 0.87) suggested that the presence of a hydrogen bond acceptor, one negative atom, two aromatic rings, and three hydrophobic groups plays a vital role in the binding of an inhibitor of FFAR-4. These pharmacophore models allowed searches for novel FFAR-1, PPAR-G, and FFAR-4 triple inhibitors from multi-conformer 3D databases (Asinex). Finally, the twenty-five best hits were selected for molecular docking, to study the interaction of their complexes with all the proteins and final binding orientations of these molecules. After molecular docking, ten hits have been predicted to possess good binding affinity as per the Molecular Mechanics Generalized Born Surface Area (MM-GBSA) calculation for FFAR-1, FFAR-4, and PPAR-G which can be further
148 investigated for its experimental in-vitro/in-vivo anti-diabetic activities.

Keywords: Diabetes, PPAR-G, FFAR-1, FFAR-4, ADMET, Docking, Virtual Screening

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CG1: Genome conformational and functionality changes induced by p53 mutation in data mining exercise

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Abstract

The classical school of thought about chromatin organization (CO) is: DNA-histones forming nucleosomes, which yields higher order structures binding to nuclear scaffold, compartmenting the genome into coregulated chromatin loops. In this model of CO, proteins called Scaffold Matrix Attachment Region binding proteins (SMARBPs) play a crucial role in securing chromatin loop boundaries with the nuclear scaffold. Whereas, the modern understanding of chromosome territories is: nucleosomes assemble to form loose unordered groups called clutches that further yields chromatin nanodomains (CND) and coregulated topologically associating domains (TADs). Transcription factor CCCTC-binding factor (CTCF, which is a SMARBP too) and the multiprotein complex cohesin, are crucial for TAD boundary formation. Thus, chromatin loops and the TADs appear homologous and understanding genome-wide TAD boundaries is essential for understanding genome regulation.

We have analysed ChIP-Seq data of 14 S/MARBPs earlier (https://doi.org/10.1093/nar/gkz562) out of which one of the S/MARBPs is mutant P53 which is mutated in approximately 70% of cancers, with the mutations predominantly affecting its DNA binding domain (R175, Y220, G245, R248, and R273). These mutations are reported for gain of a function making it act like SMARBP. Understanding how p53 mutations affect transcription factor activity and CO is crucial for understanding their oncogenic effects. To explore this further, we analysed ChIP-Seq, Hi-C and RNA-Seq data of normal and mutant p53 cancer cell lines. It reveals altered mutant P53 genome occupancy, CO and gene expression profiles in cancer cells. Thus, CO and genome function changes inducted by mutant P53 seems to largely contribute oncogenesis and pathobiology of cancers.

Keywords: mutant p53, TADs, Chromatin organisation (CO), HiC, RNA-Seq

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CG2: Dysregulation of metallothionein MT1 sub-types in TCF3::PBX1 pre-B-cell acute lymphoblastic leukemia

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Abstract

The translocation between chromosomes 1 and 19 t(1;19) produces the TCF3::PBX1 fusion protein, which leads to childhood pre-B-cell acute lymphoblastic leukemia (ALL). The molecular mechanism of oncogenesis, however, remains obscure. This study aims to identify the genes specifically dysregulated in TCF3::PBX1 translocation. The publicly available expression microarray datasets on ALL were used for weighted gene co-expression network analysis (WGCNA) to identify modules associated with TCF3::PBX1. The available knockdown and ChIP-Seq datasets were used to assess the direct targets of TCF3::PBX1. The WGCNA revealed a module enriched in genes involved in the metal ion stress to be positively correlated with TCF3::PBX1 with metallothionein isoform MT1 family members MT1E, MT1F, MT1G, MT1H, and MT1X as the hub genes. Of the 145 positively correlated genes, 19 were downregulated upon TCF3::PBX1 knockdown. Eleven of these 19 genes including MT1G, showed TCF3::PBX1 occupancy at the promoter. The Metallothionein 1 family has been implicated in various cancers; however, their role in t(1;19) pre-B-cell ALL has not been previously demonstrated. Our analysis effectively accounts for the cellular and population-level heterogeneity and identifies a novel mechanism for the TCF3::PBX1 action.

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CG3: Epitope Mapping in Leishmania: A Universal Vaccine Design Attempt

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Abstract

Leishmania, protozoan parasites, causes Leishmaniasis, a group of neglected tropical disease and are transmitted by infected phlebotominae sand flies. Disease pathology depends upon the Leishmania species, more than 20 species infect humans. Leishmaniasis includes 3 main forms; visceral leishmaniasis (VL), cutaneous leishmaniasis (CL) and mucocutaneous leishmaniasis (MCL). Estimated 50 000 to 90 000 new cases of VL occur worldwide annually, 600 000 to 1 million new CL. VL also known as kala-azar, the ailment may be fatal if left untreated in over 95% of cases. The disease state is characterized by irregular bouts of fever. An effective vaccine is needed for elimination of leishmaniasis but, no licensed human vaccines are currently available. Identifying key epitopes that can elicit robust immune responses, to enhance the efficacy of vaccine candidates and contribute to the development of effective immunological interventions for leishmaniasis. In the present research work three different species of Leishmania are selected. The predicted epitopes show acceptable antigenic, non-allergenic, no-toxic, non-homologs to human host whereas, it can induce immune response with CD8, CD4 T-cells and B-cells. A multiepitope vaccine comprising these epitopes can be a universal solution for preventing the selected three Leishmania species. Further experimental studies are needed to assess efficacy and safety in vivo/in vitro.

Keywords: Leishmania; leishmaniasis; vaccine; epitope prediction.

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CG4: Association of gene expression patterns with insulin resistance in children with T1DM

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Abstract

Double diabetes refers to the presence of insulin resistance (IR) in children with type 1 diabetes (T1DM), which complicates the achievement of euglycemia. The underlying molecular mechanisms for IR in T1DM remain poorly understood. The diagnosis of IR is performed using estimated glucose disposal, which offers limited insight into the pathophysiology of double diabetes. A study of molecular changes associated with insulin resistance could provide deeper understanding of the pathophysiology of double diabetes. A study cohort (n=50) was established in collaboration with HCJMRI, Pune. Blood samples were collected with consent, and peripheral blood mononuclear cell (PBMC) isolation was performed. Gene expression changes associated with IR were studied in PBMCs in children with T1DM using Weighted Gene Co- expression Network analysis (WGCNA). The RNA-sequencing resulted in sufficient amount of data with good quality score and percent alignment/assignment of reads. The WGCNA resulted in clustering of genes with high (>0.8) signed coefficient of determination. The WGCNA identified cluster/s of genes that significantly correlated (In conclusion, Gene expression changes associated with IR in children with T1DM were identified. These changes will shed light on the pathophysiology of IR and can aid in the implementation of preventive measures and development of novel therapeutic strategies. In future we will validate the identified markers in participants who are on hypoglycemic agents and healthy participants.

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CG5: Role of gut microbiota in estrogen metabolism: a potential indicator of breast cancer risk

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Abstract

Estrogen plays a crucial role in female reproductive health, bone density regulation, cardiovascular health, and the development of neoplastic diseases, including breast cancer. A key aspect of estrogen metabolism is mediated by gut microbiota-derived beta-glucuronidase (B-GUS) enzymes, which deconjugate estrogen-glucuronide complexes, facilitating estrogen reabsorption and extending its biological activity. However, the substrate specificity of distinct B-GUS subtypes in cleaving glucuronide bonds of various estrogen derivatives remains poorly understood. Further, metabolism of different classes of estrogen molecules leads to the production of multiple glucuronide compounds. Notably, the affinity of B-GUS sub-types for a given glucuronide substrate is known to differ considerably and information on the affinity of the B-GUS sub-types for the different estrogen-glucoronides is also not available. This study explores the activity of six unique B-GUS subtypes against diverse estrogen-glucuronide substrates, shedding light on their roles in estrogen metabolism and broader implications for human health. With these information, the impact of B-GUS on estrogen levels and potential contribution to breast cancer risk can be better understood and an insight will be gained of host-microbe interactions in hormonal regulation and may inform strategies for managing estrogen-related conditions.

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CG6: Monitoring Influenza A and its subtypes, RSV, and SARS-CoV-2 using wastewater-based epidemiology: a two-year longitudinal study in an Indian megacity covering omicron and post-omicron phases

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Abstract

The bourgeoning field of wastewater-based epidemiology (WBE) for the surveillance of several respiratory viruses which includes Influenza A, H1N1pdm09, H3N2, Respiratory Syncytial Viruses (RSV), Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) are of interest for public health concerns. However, there are few long-term monitoring studies globally. In this study, respiratory viruses were detected and quantified from 11 sewer sheds by utilizing Reverse Transcription-quantitative polymerase chain reaction (RT-qPCR) analysis in Pune City, India, from Jan 2022 to Dec 2023. The RNA fragments of respiratory viruses were detected in sewage samples before clinical cases reported, underscoring the potential of WBE for early detection and monitoring within the population. The Spearman correlation of wastewater viral copies was positively and significantly correlated with the clinically positive case of H1N1pdm09 (Ï□=0.55, p=1.4Ã—10-9), H3N2 (Ï□=0.25, p=9.9Ã—10-3), SARS-CoV-2 (Ï□=0.43, p=4.1Ã—10-6). The impact of public health interventions on the circulation of infectious respiratory diseases showed a significant difference in the viral load during the period when many preventing measures were carried out against the COVID-19 pandemic (restriction phase), compared to the period when there was no such preventive measures are followed (no restriction phase) for Influenza A, H1N1pdm09, H3N2, RSV with p-value.

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CG7: Construction and comparative analysis of phage-bacteria-food association networks

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Abstract

The relationship between the human gut microbiome and health is increasingly recognized, with bacteriophages (phage) playing a pivotal role in shaping microbial diversity and functionality. This study aims to investigate the complex interactions between gut phages and bacteria with an additional focus on bacteria communities found on food. Variety of databases like National Centre for Biotechnology Information (NCBI), the Genome Taxonomy Database (GTDB), and the Food microbio net were used to obtain the genome sequences and other metadata. State of art bioinformatics methods were used to predict the associations between the phages and bacteria using computational models that rely on their genome information. The network resulting from such associations seeks to identify patterns and establish connections between the bacterial and phage communities in the gut and those introduced through the consumed food. This network was deployed in Neo4j consisting of 10948 bacteria and approximately 8000 phages allowing for a robust exploration of the associations and dynamics within the human gut ecosystem. Various properties pertaining to the phage, bacteria and food items were also included to enrich the knowledgebase capabilities for improved querying. Furthermore, we explore the potential of predictive techniques to model novel phage-bacteria interactions, aiming to create a comprehensive knowledge graph that elucidates these relationships. This research underscores the critical need for innovative approaches to combat antibiotic resistance and enhance our understanding of the gut microbiome's role in health and disease, paving the way for future therapeutic strategies that leverage phage therapy and dietary interventions.

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CG8: Identification of symptomatic markers for schizophrenia in peripheral blood in the indian population

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Abstract

Schizophrenia (SCZ) is characterized by delusions and hallucinations, and the severity of the symptoms is estimated using Positive and Negative Syndrome Scale (PANSS). The treatment strategies such as the use of antipsychotics affect the positive symptoms while the others remain relatively less affected. Symptom-based molecular markers will enable us to understand the pathophysiology of the disorder. The review of literature identified studies that have performed targeted analysis or have correlated only with positive and negative symptoms. We performed blood-based transcriptomic profiling to identify gene cluster/s that correlate with all symptoms for their severity on PANSS. The study was conducted on a multi-centric cohort of 20 SCZ participants. The raw counts obtained from RNA-sequencing of the PBMCs isolated were subjected to the WGCNA. The gene clusters with similar expression pattern were identified and those significantly correlated with the severity of the SCZ symptoms were subjected to gene ontology and hub gene analysis. The RNA-sequencing data showed satisfactory quality. The WGCNA resulted in clustering of genes with high (>0.8) signed coefficient of determination. Several modules significantly (p.

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CG9: Exploring Somatic Mutations in Circulating Cell Free DNA

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Abstract

The detection of somatic mutations is critical for understanding tumor progression, monitoring tumor dynamics detect resistance to treatment, and identifying actionable mutations in lung cancer patients. Analysis of circulating cell-free DNA (cfDNA), released from tumor cells into the circulation, offers a minimally invasive method to assess these somatic mutations. However, low sensitivity of cfDNA analysis, due to the often-minimal presence of tumor-derived cfDNA, poses a challenge and can lead to false negatives. A potential solution to this low sensitivity of cfDNA analysis is the use of high-depth sequencing. In this study, we conducted high-depth (10,000X) next-generation sequencing of circulating cell free DNA (cfDNA) extracted from the plasma samples of lung cancer patients. The tumor DNA for the same lung cancer patients had been sequenced for actionable mutations. Our analysis demonstrated 100% concordance for single nucleotide variants (SNVs), 80% concordance for insertions and deletions (indels), and 71% concordance for gene fusions. Additionally, a comprehensive examination of somatic mutations revealed several low-frequency somatic mutations, which may provide valuable insights into the clinical characteristics of the patients.

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CG10: Novel Link Between EMP3 Overexpression and Oxidative Phosphorylation in Metastatic Melanoma

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Abstract

Background
Cancer-associated fibroblasts (CAFs) critically modulate tumor progression and immune response in melanoma. However, the molecular mechanisms linking CAF-derived prognostic markers to tumor-driving pathways remain unclear. This study aims to identify CAF-associated prognostic signatures and their relationship with critical tumor pathways in metastatic melanoma.
Methods
We analyzed TCGA-SKCM (n=452) datasets along with GTEx(n=200) and GSE15605 to identify CAF-related prognostic biomarkers using Cox regression and LASSO regression. Gene Set Variation Analysis (GSVA) was performed across 18 pathway sets to investigate CAF-pathway associations. As the CAFs have a potential role in immune cell response, therefore we assessed immune cell infiltration using CIBERSORTx and calculated tumor microenvironment (TME) scores using ESTIMATE. Correlation analysis identified associations between prognostic markers and dysregulated pathways. Response to immunotherapy was predicted by TCPA for both PD-L1 monotherapy and combined immune checkpoint blockade.

Results
We identified five prognostic biomarkers (EMP3, FLNC, MMP9, PEAR1, TGM2), from which EMP3 is highly overexpressed in CAFs and strongly linked to OXPHOS activity ($r = 0.72$, $p < 0.001$) with poor survival. High-risk patients experienced reduced immune cell infiltration and lower TME scores, indicating an immunosuppressive microenvironment. Importantly, the CAF predictive score showed positive response to PD-L1 monotherapy and combined immune checkpoint blockade (PD-L1 and CTLA-4).

Conclusion
This study reveals a novel EMP3-OXPHOS axis in metastatic melanoma. It correlates with immunosuppressive TME characteristics and may serve as both a prognostic indicator and predictive biomarker for immunotherapy response. These findings suggest targeting the EMP3-OXPHOS axis could be a therapeutic strategy for high-risk melanoma.

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CG11: Do antibiotic resistant bacteria in wastewater correlate with clinical types? A case study of escherichia coli in Pune, India

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Abstract

Antimicrobial resistance (AMR), particularly carbapenem-resistant Escherichia coli, poses a growing health threat. This study explored antibiotic-resistant E. coli in wastewater from 11 sewage treatment plants in Pune, India, between October 2023 and May 2024. We used selective media, disc diffusion, Vitek2Compact, whole genome sequencing (WGS), and real-time PCR to identify resistance patterns and genes, including blaNDM, blaOXA-like, and ESBL genes (CTX-M, SHV).

The study revealed a high prevalence of carbapenem-resistant E. coli in wastewater, with ST361 identified as the most frequent sequence type (32.25%). These isolates exhibited multidrug-resistant profiles and virulence genes comparable to clinical strains. Genomic results strongly correlated with phenotypic antimicrobial susceptibility testing.

The findings highlight the role of wastewater as a reservoir for clinically significant AMR bacteria and suggest that urban wastewater surveillance can bridge environmental and clinical AMR tracking. Such monitoring provides critical insights into resistance trends and informs public health strategies. Continuous surveillance is essential for developing effective interventions and mitigating AMR risks.

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CG12: Placental miRNA profiling in Assisted Reproductive Technology pregnancies pathway analysis

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Abstract

Background:
Infertility is a growing concern in India, and Assisted Reproductive Technology (ART) has emerged as a crucial solution. However, ART procedures are associated with placental dysfunction that can have long-term health effects for the children. We aimed to identify differential microRNAs in the placenta of women conceived by ART procedures and explore its role in fetal development using pathway analysis.

Methodology:
64 pregnant women who underwent ART procedure and 93 pregnant women with natural pregnancy (Non-ART group) were included in the study. Qiagen miRCURY LNA PCR Array was used to identify differential miRNAs from placental samples using qRT-PCR. Pathway enrichment analysis was performed for differential miRNAs using Enrichr integrated within the ShinyGO v0.80.

Result:
Placental expression of 11 miRNAs of the 28 tested miRNAs were different (5 upregulated and 6 downregulated) in the ART group. Pathway Enrichment Analysis revealed that up-regulated miRNAs are associated with pathways such vasculature development and down-regulated miRNAs with xenobiotic stimulus, stress-activated MAPK cascade, circadian rhythym, insulin stimulus and secretion, cellular response to oxygen levels and fibroblast proliferation. Validation of miRNAs on a larger sample size, demonstrated that miR-30c-5p and miR-140a-5p was downregulated in the ART group as compared to non-ART group. miRNA-mRNA target network analysis revealed that these miRNAs target 58 genes that were associated with regulation of VEGF receptor signalling pathway, glomerulus vasculature development, long chain fatty-acyl-CoA biosynthesis and apoptosis.

Conclusion:
This study identified two essential miRNAs (miR-30c-5p and miR-140a-5p) associated with ART procedures that regulate fetal growth and development.

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CG13: DapB is a conserved target for tackling antimicrobial resistance in Mycobacterium tuberculosis

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Abstract

Tuberculosis (TB) remains a major global health issue, with growing challenges posed by drug resistance, highlighting the urgent need to identify new drug targets. This study examined the conservation pattern of the dapB gene, which encodes dihydrodipicolinate reductase, a key enzyme in the lysine biosynthesis pathway of Mycobacterium tuberculosis (Mtb). This pathway is absent in humans. Drug susceptibility testing was performed on 72 Indian clinical isolates of Mtb using standard anti-TB drugs. It was found that 9.73% of isolates were multidrug-resistant. Spoligotyping revealed a complex genetic landscape, with Beijing origin strains being the most prevalent (30.56%). The dapB gene was amplified from all 72 clinical isolates, sequenced, and analysed for mutations. Further, the genomic data of 112 isolates from the BV-BRC database were also analysed. Sequence analysis identified a single DapB mutation, L65I, among clinical isolates. Analysis of BV-BRC isolates revealed an additional mutation in DapB, S89L. The mutations were mapped on the surface of the protein, and were found to be more than 10 Ã… away from the active site. Further, 100 ns molecular dynamics (MD) simulations were performed in triplicate for the native and mutant proteins to assess the impact of mutations on protein structure and function. MD simulations demonstrated no significant difference in the overall structure or the binding pocket volumes between the native and mutant proteins. This study highlights the potential of DapB as a conserved drug target for future drug development efforts aimed at tuberculosis.

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CG14: Antimicrobial Resistance Pattern Across Maharashtra

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Abstract

Antimicrobial resistance (AMR) poses a growing threat to public health, with urban wastewater serving as a critical reservoir for AMR genes and pathogenic microorganisms. This study aims to profile AMR patterns across three key regions in Maharashtra, Indiaâ€"Western Region, Mumbai Region, and Central Regionâ€"to identify specific AMR-related pathogens and drug resistance genes prevalent in these areas.

Samples were collected weekly from open drains in 23 Class-I cities across Maharashtra, covering a diverse range of urban settings from the Western, Mumbai, and Central regions. From December 2022 to May 2023. Using high-throughput sequencing and advanced bioinformatics pipelines, AMR gene abundance was quantified.

Distinct patterns were observed across the three regions, each exhibiting unique indicator taxa linked to specific AMR profiles. The Western Region was primarily associated with hospital-related bacterial taxa, significantly contributing to the dissemination of antimicrobial resistance. In contrast, the Mumbai Region was characterized by industrial and aquatic bacteria, while the Central Region was predominantly dominated by taxa commonly associated with fecal contamination and AMR genes. All three regions demonstrated a high prevalence of multidrug resistance, as well as resistance to MLS, beta-lactam, tetracycline, and bacitracin. The analysis indicated that different resistance groups exhibited distinct patterns across drug classes.

This study provides a comprehensive regional comparison of AMR patterns in Maharashtra, revealing significant variations in pathogen prevalence and AMR gene abundance across the Western, Mumbai, and Central regions. The distinct associations between specific bacterial taxa and AMR profiles highlight the critical role of local factors.

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CG15: Genomic cartography of Ventricular Septal Defects using NGS approach: Is there any impact of Anesthesia?

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Abstract

Background:
Ventricular Septal Defects (VSDs) are commonest Congenital Heart Defects (CHDs) contributing to 20-25 % of CHDs1. Multistage open heart surgeries and complex prognosis are common complications in VSD, highlighting need to reveal molecular basis of VSD to benefit genetic counseling and early diagnostic strategies. Here, we evaluate potential effect of anesthesia on genomic landscape to standardize the sample collection regime.
Methodology:
4 blood samples from 2 VSD patients were collected pre and post anesthesia. DNA and RNA library preparation was performed using KAPA Hyperplus Kit & KAPA RNA HyperPrep Kit respectively. DNA methylation analysis was done using NEBNext®Enzymatic Methyl-seq Kit (New England Biolabs). NGS was performed using Illumina NovaSeq X Plus at Strand Life Sciences.

Results:
Quality control assessments yielded high-quality DNA (Average 55.5 ng/µL; DIN: 8.3 and RNA (Average 85.34 ng/µL; RIN: 6.175). All samples passed library QC. 50 genes variants were recorded; increase/decrease in number of variants was not consistent across 2 sample sets. These included genes coding for key transcription factors (24) eg., CRELD1, BCL9, GATA4, etc., 10 cell signaling & adhesion molecules, 15 embryonic development & morphogenesis and 8 signaling & developmental pathway components important in VSD etiology. 104 upregulated and 127 downregulated genes in DEG analysis using EdgeR; did not belong to above variant panel. Except sporadic regions, no significant variation observed in genome-wide average methylation pre & post anesthesia.

Conclusion:
This proof-of-concept analysis showed insignificant impact of anesthetic drug in NGS analysis, yet more samples are needed to deduce any pattern.

References:
1. Rao PS, Harris AD. Recent advances in managing septal defects: ventricular septal defects and atrioventricular septal defects. F1000Res. 2018;7:F1000 Faculty Rev-498.

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CG16: Wastewater based epidemiology of SARS CoV 2 and Antimicrobial Resistance

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Abstract

Introduction:
Wastewater-based epidemiology (WBE) has emerged as a powerful tool for monitoring and tracking public health concerns, including infectious diseases such as COVID-19 and antimicrobial resistance (AMR). CSIR-National Chemical Laboratory (CSIR-NCL), Pune, has been engaged in wastewater surveillance since Aug 2021, and the Rockefeller Foundation,
USA, is funding the study.

Materials and methods:
In this study, we collect wastewater samples from the inlet of eleven sewage treatment plants (STPs) such as New Naidu, Old Naidu, Tanajiwadi, Vitthalwadi, Erandwane, Kharadi, Mundhwa, BhairobaNala, Baner, Bopodi and CSIR -NCL inbuild Phytorid STP. Collected samples is processed for RNA extraction and analyzed using reverse transcription- quantitative polymerase chain reaction (RT-qPCR) to quantify the SARS-CoV-2 RNA in
wastewater. Amplicon sequencing using Illumina platform is utilized for tracking virus genomic sequences to improve community prevalence estimates and detect emerging SARS-CoV-2 variants.

Results:
We regularly inform decision-makers about the presence of SARS-CoV-2 and the prevalence of any new variants in wastewater. In the context of AMR, WBE offers a valuable means to assess the prevalence and spread of antimicrobial resistance in a population. We started the analysis of genetic markers associated with AMR in wastewater samples from Dec 2022, using Nanopore-based shotgun sequencing. WBE data provides insights into the overall level of AMR in a community or region, facilitating the identification of hotspots and tracking
changes over time. Such information is essential for informing antimicrobial stewardship programs and shaping public health policies to mitigate the impact of AMR.

Conclusion:
Our study provides real-time and comprehensive insights into the presence, prevalence, and dynamics of COVID-19 and AMR in wastewater.

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CG17: Comprehensive genomic profiling of 1,000 Indian cancer genomes identify opportunity of precision medicine: a retrospective cohort study

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Abstract

Cancer patients with targetable biomarkers show much better responses to molecularly guided therapy. Global genomic profiling has catalogued novel biomarkers and driver genes in developed nations, enabling tailored therapeutic strategies. However, Indian ethnic diversity is poorly represented in such global genomic studies. This study aims to determine the landscape of molecularly targeted therapeutics using comprehensive genomic profiling to identify novel therapeutic opportunities. We attempted genomic characterization of 1000 Indian patient samples across 27 cancer types using whole exome and whole transcriptome sequencing. We developed an integrated genomics analysis computational pipeline and a clinical inference tool ClinOme to identify molecularly guided therapeutics. We identify recurrent high tumor mutation burden (TMB), microsatellite instability, and high PD-L1 expression in multiple cancers. Furthermore, we observe cancer hallmark genes such as TP53 (40 %), PIK3CA (13 %), CDKN2A (12 %), KRAS (8 %), EGFR (7 %), BRAF, RET, ERBB2, MET, ALK, FGFR3, KIT, STK11, FGFR2, ERBB3 at below 5 % frequency in Indian cohort. Altogether, about 42 % of Indian patients harbor therapeutically relevant alteration. However, we observe that only 8 % of Indian patients have access to all therapeutic options based on DCGI approvals. Largely, our study provides strong evidence for disproportional somatic molecular biology associated with ethnic descent, further underscoring novel therapeutic opportunities in one of the world's largest ethnic populations.

Keywords: Pan-cancer, Indian ethnicity, genomic profiling, clinical and therapeutic markers, computational tools.

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CG18: Evolving proteins towards acquiring novel functions

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Abstract

Spontaneous mutations occurring in DNA sequences results into nucleotide sequence change though these mutation may or may not result into protein sequence change. This probable chance of protein sequence change depend upon the nature of mutation if either it is synonymous or non synonymous. Ratio of rates of non synonymous to synonymous mutation give an idea if that mutation is getting positively selected by nature purifying in nature. Studying these ratio about a protein is important to reveal the natural intention about an evolving protein molecule. Evolution of specific sequences in signalling molecules indicate acquisition of novel function by the protein or transcription factor. This study depicts the positive selection of a transcription factor and its neofunctionalization after a gene duplication event.

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CG19: Exploring the Pan-Genomic Landscape: Unveiling Novel Colistin Resistance Determinants Beyond the Known Antibiotic Resistance Paradigm

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Abstract

In response to the escalating challenge of antimicrobial resistance (AMR), we have developed a framework for systematic post-pangenome analysis to elucidate the genetic factors underpinning microbial phenotypes. Utilizing 430 clinical isolates of Acinetobacter baumannii (22 colistin-resistant and 408 susceptible) as a case study, we analyzed pan-genome matrices comprising 24,221 gene clusters. By encompassing the entire gene repertoire of A. baumannii, including 22,774 accessory genes, the systematic analysis provided a comprehensive perspective on bacterial genetic diversity. A central aspect of our approach is the identification of characteristic accessory genes. Resistant genes are defined as those present in at least 60% of resistant isolates (≥14 of 22) and fewer than 40% of susceptible isolates (<163 of 408). Conversely, susceptible genes are those present in at least 60% of susceptible isolates (≥245 of 408) and fewer than 40% of resistant isolates (~9 of 22) (user defined threshold based on the size of the sample). These prevalent accessory genes are hypothesized to play crucial roles in enabling certain clinical isolates to resist antibiotic treatment. Additionally, we investigated interactions between these characteristic accessory genes and core/accessory genes which are already known drug resistance (DR) determinants, uncovering potential synergistic mechanisms that confer resistance. One significant challenge addressed by this approach is the lack of comprehensive protein-protein interaction data essential for understanding DR mechanisms. To overcome this, we estimated gene occurrence across resistant and susceptible isolates and analyzed these patterns within their regulatory networks based on gene co-occurrence matrices. Employing community clustering algorithms on Jaccard similarity coefficient matrices derived from both resistant and susceptible isolates, our approach identifies tightly-knit clusters of functionally related genes. Furthermore, by comparing these matrices, we pinpoint gene pairs entirely absent in either resistant or susceptible isolates, highlighting potential novel resistance determinants. By systematically analyzing both core and accessory genomes and their interactions, our study enhances the understanding of AMR and provides avenues for innovative solutions to combat antibiotic-resistant pathogens by identifying putative novel resistance determinants.

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CG20: Exploring Gut Microbiome Variability in Indian Grey Wolves (Canis lupus pallipes) Relying on Anthropogenic Subsidy: A Frame work from Baseline Data

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Abstract

The Indian Grey Wolf (Canis lupus pallipes) is an endangered species facing significant threats from anthropogenic pressures, including habitat loss, human-wolf conflict, and disease transmission from feral dogs. This report is a part of a study that investigates the impact of these pressures on the dietary habits and gut microbiome diversity of the Indian Grey Wolf, which is listed as Vulnerable in CITES Appendix II. Understanding dietary shifts in response to anthropogenic subsidies is crucial for conservation efforts, health monitoring, and mitigating human-wolf conflicts.

In this study, we employ a non-invasive approach combining scat analysis with metagenomics to assess seasonal variations in diet and gut microbiome composition. Python is utilized for the extraction and processing of microbiome functioning data, while R is employed for data analysis and visualization, allowing for clear insights into dietary preferences and microbial diversity.

Preliminary findings suggest that there is an increased reliance on anthropogenic food sources, such as dumped poultry carcasses or any other food sources that may lead to a shift away from natural prey like chinkara and blackbuck. This study revealed the presence of members of Ruminococcaceae, Blautia, Prevotella spp., Romboutsia, all know for digestion of dietary fibres and complex carbohydrates, in the gut microbiome.

This dietary change not only affects the wolves' ecological role but also raises health concerns due to increased exposure to diseases. The results will provide valuable information for conservation strategies aimed at protecting the Indian Grey Wolf and promoting coexistence with local communities.

Ultimately, this study highlights the importance of integrating bioinformatics in wildlife research, utilising interdisciplinary collaboration, offering a comprehensive framework from the baseline data to understand gut microbial functioning in relation to dietary shifts. By addressing these critical issues, we aim to contribute to effective conservation practices that ensure the survival of this vulnerable species in an increasingly human-dominated landscape.

Keywords: Indian Grey Wolf (Canis lupus pallipes), Dietary shift, Gut microbiome, Scat analysis, Metagenomics, Anthropogenic pressure, Conservation strategies.

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AS1: Variational Quantum Eigensolver for Molecular Dynamics: A Benchmark Study

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Abstract

Molecular Dynamics (MD) simulations are widely used to study the physical behavior and movements of atoms and molecules over time, providing valuable insights into the dynamic evolution of complex molecular systems. However, as the molecular complexity increases, traditional MD simulations become computationally intensive, requiring significant time and resources. In this context, quantum computing could offer a promising solution, particularly through the Variational Quantum Eigensolver (VQE) algorithm. VQE is a hybrid quantum-classical approach that can efficiently solve quantum chemistry problems by finding the ground state energy of molecular systems. We have done simulation using qiskit simulator platform . Benchmarking studies on molecules like H2, LiH, and H2O, C2H5OH, N2, CH4 taking time 102.2135sec, 172.1715sec, 413.2669sec, 375.9453sec. 5414.3795sec, 6263.5310sec. The result demonstrates that as the complexity of the molecule increases the qubit requirement also increases. The number of qubits required in VQE is directly proportional to the number of electrons and orbitals in the molecule. This requires complex quantum computer with more number of qubits. The benchmarking results show that as molecular complexity increases, the VQE algorithm's qubit requirement rises, with simulation times ranging from 102.2135 seconds for H2 to 6263.5310 seconds for CH4. This indicates the need for more advanced quantum computers to handle larger, more complex molecules efficiently.

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AS2: Predicting Surface Protein Expression in Single Cells: A Machine Learning Approach

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Abstract

Advances in single-cell genomics have enabled the simultaneous measurement of multiple molecular modalities, such as RNA expression and surface protein levels, within individual cells. CITE-seq (Cellular Indexing of Transcriptomes and Epitopes by sequencing) provides a multi-modal framework to study the interplay between transcriptomic and proteomic data, but analyzing and integrating these datasets remain challenging due to sparsity, noise, and batch effects.

In this work, the Kaggle Multimodal Single-Cell Integration dataset to benchmark machine learning models for predicting surface protein levels (ADT data) from RNA expression profiles (GEX data) is used. The dataset includes 300,000 CD34+ hematopoietic stem and progenitor cells (HSPCs) collected at five time points from four human donors, capturing the dynamic development of bone marrow stem cells into mature blood cells. The goal is to predict how DNA, RNA, and protein measurements co-vary during this differentiation process. Advanced machine learning models are employed and the model performance is evaluated by computing the correlation between ground-truth surface protein measurements and predicted values across diverse cellular states. The approach also incorporates advanced techniques to handle technical noise, feature sparsity, and batch effects, enabling accurate integration of multimodal data. The task bridges the gap between transcription and protein production, highlighting the functional outputs of gene activity during blood cell development.

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AS3: TERP: Machine Learning-based prediction of TCR-peptide binding specificity

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Abstract

Adaptive immunity relies on the recognition of peptide-MHC complexes by T-cell receptors. A highly diverse TCR repertoire is developed by genetic recombination estimated in the range of 1015 up to 1061. TCR diversity is exhibited in CDR regions that contact pMHC and determines the specificity of TCR-pMHC. Although crystal structures of TCR-pMHC complexes provide insight into mode of recognition, the availability of sequences of cognate TCRs for a given pMHC has been the major limiting factor in deciphering recognition specificity. Profiling of TCR-pMHC recognition remains a challenging task in immunology, and ability to predict TCR-pMHC binding provides the opportunity to develop immunotherapies and new-vaccines. Recent advancements in tetramer-based single-cell-TCR sequencing techniques provide valuable information about TCRs, peptides, and MHCs. Moreover, the advent of artificial intelligence and machine learning techniques allows the prediction of TCR-pMHC binding based on CDR3 and peptide sequences from publicly available datasets such as VDJdb, IEDB, and McPAS-TCR. The TERP (TCR-Epitope Recognition Prediction) model was developed using paired TCR-peptide (pan-specific) sequences, employing the classical Random-Forest algorithm and di-peptide features. The TERP model has shown better predictive performance with the AUC of 0.83 and 0.80 in TCR-Split (80:20 split) and Strict-Split (less-frequent peptide-TCR pairs in test set) models, respectively. Notably, TERP model showed generalizability in predicting unseen TCR-peptide pairs, whereas other published models failed to predict. For unseen SARS-CoV-2 peptide-specific TCR datasets, the ROC-AUC and PR-AUC were found to be 0.77 and 0.80, respectively. In addition, we have developed a user-friendly web portal for TCR-pMHC binding prediction (http://www.nii.ac.in/TERP).

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AS4: Development of a GUI for GROwin Software to Streamline Molecular Dynamics Simulation

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Abstract

We introduce a graphical user interface (GUI) developed specifically for GROEin software to streamline and enhance the workflow of molecular dynamics (MD) simulations. This user-friendly GUI is designed to remove the technical barriers associated with command-line operations, allowing users to set up, execute, and analyze MD simulations in an efficient and intuitive manner. By simplifying the configuration and execution of MD tasks, the GUI significantly reduces the learning curve for new users while improving productivity for experienced researchers. The tool automates key aspects of the simulation process, from input file preparation to visualization of results, offering robust analysis features like tracking simulation progress, detailed reports, and customizable visualizations. With its integrated design, this GUI promotes faster, more reliable simulations and ensures that researchers can focus on scientific insights rather than software complexities, making it an essential tool for a variety of MD applications in computational biology, chemistry, and materials science

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AS5: AI/ML-guided prediction of host-virus protein-protein interactions

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Abstract

Viruses are intracellular parasites that depend on host protein interactions to survive. Understanding these protein-protein interactions (PPIs) is essential for uncovering infection mechanisms and developing therapies. While experimental techniques and atomic-resolution 3D structure analyses offer precision, they are time-consuming. Computational methods, such as interlog mapping and interaction interface conservation, provide quicker predictions based on homolog information. However, new viruses with limited representation in existing host-virus PPIs challenge these approaches. Machine learning (ML) addresses this gap by automatically extracting features from known PPI datasets. ML is particularly effective for novel viruses, identifying conserved PPI-related features and enabling efficient automated predictions. Hence, we have attempted to develop a ML model for identifying the human-virus PPIs using the public datasets emphasising SARS-CoV-2-associated datasets. For the ML model development, we utilized various algorithms (Random-Forest, CNN, etc) and feature vectors (di-peptide, tri-peptide frequency, bioembedding, etc). 5-fold cross-validation was performed for the training data to check the model's generalizability, and we achieved a ROC-AUC of 0.95 with tri-peptide frequency and random-forest algorithm. Also, to emphasise the use of our ML based method in case of new viruses, we have used training datasets devoid of SARS-CoV-2 information and tested on SARS-CoV-2 dataset achieving ROC-AUC of 0.7 and 0.8 for di-peptide and tri-peptide frequency, respectively. This analysis can facilitate the rapid collection of extensive host-virus PPI data for emerging viruses during pandemics.

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AS6: Development of algorithms for prediction of MHC binding peptides using ML methods

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Abstract

Prediction of MHC binding peptides is the cornerstone in the development of computational immunology. This has applications in almost in all fields of immunology especially in vaccine designing, immunotherapy, immune evasion response studies. MHCs are antigen presenting molecules. The MHC molecules mainly belong to two classes. The class I molecules are responsible for displaying antigens that are already located inside the cell to cytotoxic t cells, while class II molecules engage in presenting peptides or antigens derived from outside the cell to helper t cells. The MHC molecules found in humans are referred to as HLA molecules. Machine learning is a division of Artificial Intelligence. It employs a method where we train the system using a specific dataset that is typically obtained through experiments and utilize it on a broader dataset to generate a predictive model. In this study we try to make allele specific models for MHC binding peptide predictions. Allele specificity is important as in pan allele studies there is a lot of noise and the data available for all alleles is not comparable. The machine learning model have different types out which support vector machines and random forests are the one that are used in this study. SVM excels in handling high-dimensional data and identifying non-linear patterns, while RF provides robustness through ensemble learning. The models used features like Length of the peptide, isoelectric point, molecular weight, hydrogen bonding pattern and many more like this for this study. Through extensive performance evaluation, the study demonstrates that both SVM and RF can achieve high predictive accuracy, with insights into their respective strengths in handling diverse data types.

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AS7: Search Engine for Omics data: from sequencing to quick analysis

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Abstract

An expansion in the production of single-cell data from different modalities has expedited the need for search engines. In this poster, I'll showcase the capability and usefulness of such a search engine in facilitating actionable inference from big data. I'll also shed light on the underlying computational frameworks of the tools.
CellAtlasSearch v2:
CellAtlasSearch uses GPU computing and Big Data mining techniques to address this need in a scalable manner. Users can query with one or multiple single-cell expression profiles to retrieve the top matches from a large database of single-cell and bulk expression profiles, along with relevant meta-information.
Studying single cells using CellAtlasSearch v2, allows users to query single-cell expression profiles to retrieve matching single-cell or bulk expression data from over 2000 different studies. CellAtlasSearch v2 Pipeline in the entire web server is based on the GPU framework. Expression profiles are stored as hash codes obtained through LSH. Like-samples are archived in the same bucket. Query expression data is first converted into hash code and then mapped to one of the buckets. Users can query one or more single-cell transcriptomes. Additional functionalities have been added to the updated version, such as â€˜cell healthâ€™ indicators and trace of diseases. This update includes an R-package so that the user can use the functionalities for custom downstream analysis.

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AS8: Classification of Mononuclear Copper Binding Sites Using Machine Learning-Based Clustering

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Abstract

Copper is an essential metal ion involved in various metabolic processes, including electron transport, oxygen transport, and reduction reactions. Copper binding proteins are traditionally classified into groups based on ligand composition, geometry of the metal center, and characteristic spectroscopic properties, such as the type 1 and type 2 mononuclear centers. However, these classifications often overlook the structural aspects and complex nature of the binding sites. In this study, we aim to analyze mononuclear CuÂ²â°binding sites from the experimentally resolved protein structures using machine learning algorithms. We examine a wide range of features, including residue types, coordinating atoms, their counts, residue properties, coordination geometry and secondary structure elements. Not surprisingly, the larger clusters correspond to the previously defined type 1 and type 2 sites. However, preliminary findings indicate significant complexity in CuÂ²â° coordination, challenging existing classifications. By employing various clustering algorithms, we have uncovered new patterns and classifications that may reveal previously unrecognized types of CuÂ²â° binding sites. Surprisingly, we have identified sites resembling zinc binding sites, such as 4-Cys and 1-Glu,1-His sites, raising questions about the factors determining the specificity of divalent metal ions. We have developed a comprehensive classification system that integrates structural insights and sequence motifs, enhancing our understanding of CuÂ²â° binding sites. Furthermore, we will explore predictive modeling techniques to identify CuÂ²â° binding sites within proteins, enhancing our understanding of these crucial metal-binding proteins.
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AS9: Auto-NAMD: A stand-alone GUI tool for NAMD Simulations

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Abstract

Molecular dynamics (MD) simulations are essential for understanding molecular interactions at the atomic level in computational biology and material science. However, the learning curve associated with setting up and execution often deters researchers and users without programming expertise. To address this challenge, we bring forward an intuitive Graphical User Interface (GUI) based tool designed for setting up molecular dynamics simulations using a widely adopted Nanoscale Molecular Dynamics (NAMD) program. Auto-NAMD is designed with modularity and ease to cater to users of varying expertise, from novice to experienced researchers. It allows users to configure key simulation steps, such as minimization, heating, and equilibration, through a simple tabbed Graphical interface. This tool enables customizing input parameters like cell basis vectors, cell origin, and periodic boundary conditions. Advanced features such as water wrapping and DCD file browsing enhance overall functionality. It nullifies manual scripting thus reducing the setup time and likelihood of errors, by automating routine tasks. Auto-NAMD democratizes molecular dynamics simulations, allowing users of research backgrounds to focus on scientific discovery rather than technical details. Auto-NAMD provides an accessible, efficient, and reliable platform for MD simulations, fostering interdisciplinary advancements in computational research.

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AS10: Target.AI : Drug sensitivity prediction for targeted cancer therapy

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Abstract

The aberrant alteration in genes, such as EGFR, resulting from somatic mutations, is associated with driver phenotype, making them a critical target in cancer therapy. This study aims to predict the response of Tyrosine Kinase Inhibitors (TKI) in cancer patients through an easy-to-use web server utilizing artificial intelligence (AI). We developed an automated and scalable server, including modelling, molecular docking, and molecular dynamics (MD) simulations to elucidate the interactions of EGFR mutants (N ~ 700) with TKIs. These EGFR mutation models, molecular docking scores, and MD simulation reveal an interesting correlation between in-silico observations and clinical TKI sensitivity. We developed a machine-learning model utilizing features of protein sequence, structure, and dynamics. The ML model achieves an accuracy of 93.7 % and an F1 Score of 97.9 % for the TKI-sensitivity prediction for mutations occurring in the kinase domain of EGFR. Using this model, we characterize the sensitivity of novel EGFR kinase domain mutations previously considered variants of unknown significance (VUS). We present a new AI model capable of non-linear interpretation from complex data, allowing us to predict the sensitivity of novel EGFR VUS observed during clinical follow-up of cancer patients. The AI model is running over an easy-to-use web-server enabling biologists and clinicians to easily utilize it in their practice. Further refinement and clinical validation of this model may provide valuable solutions to predetermine the drug sensitivity of patients in clinics.

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AS11: Machine learning models to assess the impact of smoking on alcoholic liver disease

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Abstract

Alcoholism and smoking are major habits concerning public health. Alcohol is an important risk factor by WHO for disability and death in population aged between 15-49yrs. Alcohol consumption in excess causes liver disease and includes a spectrum of conditions from mild scarring to severe cirrhosis. These conditions are further reported to be exacerbated by smoking as it causes oxidative stress and fibrosis in severe disease course. The specific impact of smoking on the progression of liver disease in alcoholics is yet to be ascertained. Thus, the objective of the present study is to analyse using machine learning models if smoking and alcoholism are cumulatively enhancing liver disease. The dataset used in the present study was taken from NHANES survey for the period from 2021-2023 and included demographic, examination(Liver elastography including CAP score), laboratory(HDL-Cholesterol, Total Cholesterol, C-reactive protein) and questionnaire data (Alcohol consumption and smoking). A total of 11,900 records were curated to identify alcoholics who were smokers and nonsmokers in the age group of 40yrs and above. A total of 733 records of participants (including males and females), who were alcoholics were used for the present analysis. The resulting data sets were examined in machine learning models including Random Forest, Gradient Boosting and Support Vector Machine models. Preliminary results indicate a cumulative effect of alcoholism and smoking in liver diseases. This study is significant as it investigates the influence of smoking, a preventable risk factor, on the disease burden and mortality rate of alcoholic liver disease.

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AS12: Harnessing AI for Gut Health: Development of a Gut-Specific Chatbot Using llama3

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Abstract

Artificial intelligence (AI) and natural language processing (NLP) are transforming healthcare by enabling personalized and accessible solutions. We present an innovative chatbot specifically designed to answer gut health-related queries, built on llama3, an open-source state-of-the-art large language model (LLM). Retrained on a curated dataset of gut-specific scientific literature and anonymized patient data, the chatbot delivers accurate, reliable, and context-aware responses.
Qualitative assessments were performed to evaluate the chatbot's performance. Expert reviewers, including gastroenterologists and microbiome researchers, rated the chatbot's responses for relevance, scientific validity, and user-friendliness. The feedback highlighted the chatbotâ€™s ability to translate complex gut microbiome concepts into simple, actionable information tailored to diverse audiences. The tool proved particularly effective in educating patients about gut health, questions about their gut health reports generated by MicrobioTx, and offering lifestyle recommendations.
This chatbot bridges a critical gap between rapidly evolving scientific research and its application in gut health management. Beyond patient interaction, it holds potential for clinical support, pre-diagnostic assessments, and public health education. The retraining process emphasizes the importance of domain-specific customization in enhancing the reliability and applicability of LLMs in healthcare. By integrating cutting-edge AI with expert-reviewed qualitative evaluation, this project exemplifies how computational technologies can empower personalized medicine and advance our understanding of gut health.

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AS13: Whole Slide Imaging Annotation Using Graph-RAG and LLAMA 3.2

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Abstract

Whole Slide Imaging (WSI) plays a crucial role in high-resolution analysis of histopathological samples, enabling precise identification and annotation of structures. In this paper, we offer a Knowledge Represented in Graph-RAG and agents for reasoning for WSI data that integrates the LLAMA 3.2 with multimodal reasoning using GraphRAG. Based on visual characteristics and anatomical context, the system is intended to recognize and label WSI segments in spinal cord sections, including the anterior fissure, posterior root, and blood vessels.
SAM 2 is used for segmentation as part of the Agent's tool functionality. The LLAMA 3.2 model then uses the segmentation findings and domain-specific information in the graph to iteratively refine the labels. Additionally, it creates well-organized, comprehensive annotations for the user using structured generation using outline package. In addition to automating labeling, this integrated method enables that the system can continuously improve its predictions using the rich domain knowledge and visual context that the WSI data provides.

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AS14: Integrative omics analysis for Adrenoleukodystrophy (ALD) : The current updates and challenges

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Abstract

Adrenoleukodystrophy (ALD) is an X-linked metabolic disorder characterized by the accumulation of very long-chain fatty acids (VLCFAs) due to mutations in the ABCD1 gene. Key pathways included peroxisomal beta-oxidation, oxidative stress responses, and neuroinflammation. Genomic variant analysis highlighted novel mutations in regulatory regions of significant genes, shedding light on transcriptional dysregulation. Though its genetic basis of of Adrenoleukodystrophy (ALD) is well established, but the underlying molecular pathways and disease progression mechanisms remain inadequately characterized.

In general transcriptomic analysis involves the identification of DEGs distinguishing ALD patients from controls, implicating pathways involved in lipid metabolism, inflammatory signalling, and neuronal function while variant analysis establish relationship with disease progression and state this collectively impact in understanding the insight of disease mechanism and helping in better diagnostic and therapeutic. Recently integrative bioinformatics analysis along with predictive technologies based on Deep learning, Machine learning, NLP, AI based models and Graph neural network etc for microarray data and RNA seq have been highly encouraged by researcher to study the disease-gene associations and understanding their impact on disease progression. Most models achieved varied classification accuracy in distinguishing ALD patients from healthy controls, effectively capturing the intricate relationships within the dataset. Key features driving classification performance were mapped to critical molecular players, such as ABCD1, PEX7, and inflammatory mediators, reinforcing their roles as potential biomarkers or therapeutic targets.

In addition to predicting the effects of coding variants, omics analysis faces a number of other challenges, such as variant prediction analysis, which involves an incomplete human reference genome, a limited number of robust validated variant truth sets, and no obvious best performing algorithm.

Combining ensemble methodologies for differential expression and variant identification with the innovative application of soft computing algorithms (DL/ML based)/framework may provide important insights into the links between genotype and phenotype.

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AS15: Motor intention prediction from surface electroencephalograms: An exploratory analysis

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Abstract

Introduction

Several different approached have been tried for motor intention prediction from electrocorticograms (ECoG) with varying degrees of success. However, there is a dearth of models for prediction of the same from surface electroencephalograms (EEG). Recording from surface is non-invasive and convenient, for both the patient and the physician. Thus brain computer interfaces based on surface EEG holds greater utility. In the present study we have used an open source EEG dataset to explore the performance of a variety of machine learning & deep learning models.

Materials and methods

The Physionet motor movement EEG dataseti was used for this purpose. The dataset was recorded at 160 Hz, with labels placed according to upper limb movements (right versus left). The data was split into training (197) and validation (130 recordings). The recordings were truncated to first 3.2 seconds (512 samples) of the movement, i.e. the hypothesised time when movement is planned and neuromuscular units are recruited. ML models of increased complexity were used for exploratory analysis of the datasets, both in amplitude and in frequency domain.

Results

The best accuracy (80%) in the binary classification of motor intention (left versus right) was obtained from amplitude based analysis (after scaling), using a deep recurrent neural network (DRNN) architecture described by Roy et al (2018). Conventional ML models were found not be be suitable for the task. Interestingly, application of the same DRNN architecture on frequency domain (i.e. post fast Fourier transform) did not produce comparable results.

Conclusion

The deep recurrent neural network (DRNN) architecture applied on amplitude domain of EEG signals may hold promise for successful motor intention classification and thus contribute towards brain computer interfaces from surface recordings.

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AS16: Application of ML in identifying farthest frames from MD trajectory data in the MSM analysis

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Abstract

Molecular dynamics (MD) is a computational simulation technique used to study the physical movements of atoms and molecules. This method providing insight into the dynamic behaviour of the system. Biomolecules, such as proteins, lipids possess complex structures and perform diverse functions within living organisms and MD simulations are the main tool to understand the dynamics of it. To understand the nature of many scientific phenomena, natural or artificial, requires exploration across a wide range of spatial and temporal scales. Multiscale modelling is often used to gain scientific insights by investing computational resources appropriately across scales.
Here, we have tried to develop new ML based algorithm to extract two farthest frame i.e. most unexplored frames from given trajectory data by using MSM with PyEMMA library of python on Jupyter notebook. This tool is useful to restart simulations from the farthest frames to explore better the free energy landscape of biomolecules. The future of the work is to prepare for exascale ready automated adaptive sampling simulations tool. A case study for adaptive simulations for cancer protein is ongoing.

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AS17: Harnessing Deep Learning Docking Models for Identifying Biofilm-Inhibiting Molecules in Herbs Targeting Acute Rhinitis Bacteria

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Abstract

Machine learning (ML) methods play a significant role in analyzing the genetic diversity of tuberculosis bacilli. Early detection and diagnosis of Tuberculosis (TB), along with identifying drug resistance, are crucial for addressing the global TB burden. Genetic variations among Mycobacterium tuberculosis complex (MTBC) species are primarily characterized by single nucleotide polymorphisms (SNPs) and specific regions of deletions. In this study, we implemented a variant calling pipeline using more than 20000 publicly available whole-genome sequences (WGS) of human-adapted Mycobacterium species to identify SNPs. This pipeline included aligning sequences to a reference genome (Mycobacterium tuberculosis H37rv) using BWA and variant calling with GATK. Variants were prioritized based on their association with essential genes identified in mutagenesis experiments, non-drug resistance SNPs (SNPs not linked to drug resistance) reported by the WHO, and synonymous mutations. Lineage-specific SNPs were identified for each human-adapted lineage (1 to 6), and these selected variants were incorporated as features to develop ML models. These lineage-specific adaptations could reflect evolutionary pressures such as immune evasion or differences in metabolic pathways that benefit MTBC survival in particular human populations. Logistic Regression and Decision Tree classifiers were employed to train and test the SNP datasets. A confusion matrix was used to compare actual and predicted MTBC lineages, yielding remarkable classification accuracy (>98%) at both lineage and sub-lineage levels. This tool is a robust ML model for predicting the lineages of uncharacterized Mycobacterium species, potentially aiding in timely TB diagnostics and enhancing public health surveillance and control efforts.

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AS18: Decoding Protein-Protein Interaction Interfaces Directly from Primary Sequences with Large Language Models

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Abstract

The inter-protein interactions within a cell are essential for understanding the diverse cellular processes. A comprehensive understanding of the protein-protein interaction (PPIs) interfaces could provide valuable insights into functional analysis of the protein and its behaviour in the cellular environment. Protein sequences carry evolutionary information that provides details about their structure and function. Protein language models (PLMs) trained specifically on protein sequences learn the intrinsic patterns, structural features, and functional implications embedded within protein sequences, enabling applications like protein structure prediction, functional annotation, and interaction prediction. In our current research, an attempt is made to develop an MSA-free model by leveraging the utility and reliability of protein language models to learn protein-protein interaction (PPI) interfaces. The state-of-the-art protein language models are pre-trained on large datasets, enabling embeddings to be computed once and reused efficiently, significantly reducing the computational cost of re-training. These embeddings effectively capture critical evolutionary and functional patterns required for accurate PPI interface predictions. Additionally, we applied Parameter Efficient Fine-Tuning (PEFT), which freezes the majority of the model parameters while updating only a small subset. This approach accelerates training while still capturing essential task-specific patterns. The PLM is fine-tuned on a dataset of dimer protein sequences using a Masked Language Modeling (MLM) approach. After fine-tuning the model, we aim to utilize the learned attention heads to predict protein contact maps, which represent the spatial proximity between amino acid residues in a sequence. The spatial information learned from contact maps improves the ability of the PPI prediction model.


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GS1: Dissemination of Scientific Results: A Case for Preprints Towards Open and Inclusive Science in India

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Abstract

Preprints are complete scientific articles deposited in servers, free of cost. Preprints speed up the sharing of new findings, make scientific information freely and widely accessible, establish the priority of scientific work, boost article visibility and citation, and promote open science. There are no studies on the numbers and analysis of preprints, especially in different life sciences domains, from India. We aim to fill that gap. With concrete data and analysis, our study aims to provide recommendations on the goal of greater preprint adoption in the life sciences community in India.
The poster will present data on the current scenario of preprint usage in India through advanced data analysis and modelling, including predicting future trends and usage across various life sciences disciplines in India. Furthermore, it explores the benefits and challenges of preprint adoption in India and describes strategies for enhancing Indiaâ€™s participation in the global preprint movement, offering valuable guidance to policymakers, institutions, and researchers on leveraging preprints to accelerate scientific progress and foster collaboration.

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