I.T.S College of Pharmacy

ORGANIZES

Dr. A.P.J. ABDUL KALAM TECHNICAL UNIVERSITY
SPONSORED
NATIONAL CONFERENCE

on

Computer Aided Design Tools
for
Innovation in Pharmaceutical Sciences

CONFERENCE PROCEEDINGS

11th September, 2026

Organized by
I.T.S College of Pharmacy
Delhi-Meerut Road, Murad Nagar, Ghaziabad,
Uttar Pradesh, 201206

ABOUT I.T.S -THE EDUCATION GROUP

I.T.S – The Education Group, founded in 1995 by a charitable trust under the visionary leadership of Dr. R. P. Chadha and nurtured by Vice Chairman Mr. Arpit Chadha, has emerged as a premier academic hub. From its first campus at Mohan Nagar, it now spans four campuses across 60 acres in Ghaziabad, delivering programs in Management, Information Technology, Dental, Engineering, Pharmacy, and Physiotherapy, with advanced infrastructure, modern laboratories, hostels, and a mission to prepare nearly 8,000 globally competent professionals annually.

ABOUT I.T.S COLLEGE OF PHARMACY

Established in 2004, I.T.S College of Pharmacy, Ghaziabad, is committed to excellence in pharmaceutical education and research. The institute offers B. Pharm and M. Pharm (Pharmaceutics and Pharmacology) programs affiliated to Dr. A.P.J. Abdul Kalam Technical University (AKTU) and approved by the Pharmacy Council of India (PCI). The NBA accredited B. Pharm program reflects the institution's commitment to quality education. With a research-oriented faculty having nearly 500 publications and presentations at prestigious international conferences, the college fosters innovation, academic excellence, and global collaboration.

ABOUT THE UNIVERSITY

Dr. A.P.J. Abdul Kalam Technical University (AKTU), Lucknow, established in 2000, is a premier technical university of Uttar Pradesh committed to excellence in education, research, innovation, and skill development. With over 760 affiliated institutions, the University offers undergraduate, postgraduate, and doctoral programs in engineering, pharmacy, architecture, management, computer applications, and allied disciplines, fostering industry-oriented and research-driven education.

ABOUT THE CONFERENCE

Sponsored by Dr. A.P.J. Abdul Kalam Technical University (AKTU), this conference aims to highlight the transformative role of computational tools in pharmaceutical research and development. It will bring together academicians, researchers, industry professionals, and students to explore advances in computer-aided drug design, artificial intelligence, molecular modeling, formulation development, predictive pharmacokinetics, and Quality by Design (QbD), fostering innovation, interdisciplinary collaboration, and stronger academia–industry partnerships for a digitally empowered pharmaceutical workforce.

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Chief Patron's Message



It is a matter of immense pleasure and pride to learn that I.T.S College of Pharmacy, Ghaziabad, is organising an **AKTU-sponsored National Conference** on the theme "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences" on 11th September 2026.

In today's rapidly evolving world, technological advancements are transforming every sphere of education, research, and professional practice. Integrating digital and computational tools with pharmaceutical sciences is an important step toward fostering innovation and developing new approaches to address the challenges of the healthcare sector. Such initiatives encourage the exploration of emerging ideas and strengthen the culture of research and innovation among students and professionals.

The conference provides a valuable platform for academicians, researchers, industry professionals, and students to come together, share their knowledge and experiences, and engage in meaningful academic discussions. I am confident that this gathering will promote the exchange of ideas, encourage interdisciplinary collaboration, and inspire participants to explore new possibilities in the field of pharmaceutical sciences.

I appreciate the organising committee's efforts in selecting a contemporary and relevant theme and providing an opportunity for intellectual interaction and knowledge sharing. Such academic initiatives play a significant role in nurturing young talent and strengthening the connection between education, research, technology, and industry. I extend my heartfelt congratulations and best wishes to the organising committee and all the participants. I hope that the conference will be a rewarding and memorable academic experience for everyone associated with it.

I wish the conference every success.

Dr. R. P. Chadha
Chairman
I.T.S – The Education Group

Co-Chief Patron's Message



It is a matter of great satisfaction to know that the **AKTU Sponsored National Conference** on "**Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences**" is being organised on **11th September 2026** at **I.T.S College of Pharmacy, Ghaziabad**. The theme is highly relevant and timely, as rapid advances in computational technologies are transforming the landscape of pharmaceutical research, drug discovery, development, and healthcare.

Computer-aided approaches have emerged as powerful tools to accelerate and improve the pharmaceutical research process. Techniques such as computer-aided drug design (CADD), molecular docking, virtual screening, molecular dynamics simulation, pharmacophore modelling, quantitative structure–activity relationship (QSAR) analysis, cheminformatics, bioinformatics, and artificial intelligence and machine learning are increasingly enabling researchers to understand complex biological interactions and identify promising therapeutic candidates with greater efficiency. These technologies can reduce the time, cost, and experimental burden associated with conventional drug discovery while supporting more rational, evidence-based decision-making.

Dr A.P.J. Abdul Kalam Technical University is committed to fostering innovation, research excellence, interdisciplinary collaboration, and industry-oriented education. The University encourages the adoption of emerging technologies and promotes an academic environment in which students, researchers, academicians, and industry professionals can work together to address contemporary challenges in science and healthcare. Conferences of this nature provide an important platform for sharing scientific knowledge, presenting emerging research, exchanging innovative ideas, and establishing meaningful collaborations among academia, industry, and research organizations.

I am confident that the scientific contributions presented during this conference will provide valuable insights into the current and future applications of computer-aided technologies in pharmaceutical sciences. I hope the conference will inspire young researchers and students to embrace interdisciplinary, technology-driven approaches and contribute to the development of innovative solutions for the pharmaceutical and healthcare sectors.

I extend my best wishes for the success of this scholastic endeavour and sincerely hope that the conference outcomes will contribute significantly to advancing computational pharmaceutical research, strengthening academia–industry collaboration, and promoting innovation for the betterment of society.

Prof. Jay Prakash Pandey
Vice Chancellor
Dr. A.P.J. Abdul Kalam Technical University,
Uttar Pradesh, Lucknow

Patron's Message



It gives me great satisfaction to witness I.T.S College of Pharmacy, Ghaziabad, taking another significant step toward promoting scientific discourse and innovation by organising an **AKTU Sponsored National Conference** on "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences" on 11th September 2026.

We live in an era where technological advancements are continuously redefining how knowledge is created, shared, and applied. The growing integration of computer-aided tools and digital technologies into pharmaceutical sciences has opened new avenues for research, innovation, and problem-solving. The theme of this conference is therefore both contemporary and highly relevant to the changing landscape of science and technology.

The conference offers a valuable platform for attendees to come together, exchange ideas, explore emerging developments, and gain insights into the evolving role of technology in pharmaceutical research and innovation. Such academic gatherings are instrumental in encouraging interdisciplinary learning and fostering curiosity and innovation among young minds.

I appreciate the organising committee's efforts in selecting such a significant theme and creating a platform for meaningful scientific interaction and knowledge exchange. I sincerely hope that the deliberations during the conference will stimulate new ideas, promote collaboration between academia and industry, and motivate young researchers to explore innovative approaches in their respective fields. I extend my heartfelt best wishes to the organizing committee and all the participants for a highly successful and intellectually enriching conference.

With best wishes for the conference's grand success

Mr. Arpit Chadha
Vice Chairman
I.T.S - The Education Group

Patron's Message



It is a matter of great pleasure to note that I.T.S College of Pharmacy, Ghaziabad, is organising an **AKTU Sponsored National Conference** on the theme "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences" on 11th September 2026.

Academic institutions have an important responsibility not only to impart knowledge but also to create an environment that encourages dialogue, exploration, and continuous learning. Conferences and similar academic platforms provide opportunities for individuals from diverse backgrounds to come together, share their experiences, and collectively contribute towards the growth of knowledge.

The chosen theme reflects the growing importance of technology and innovation in shaping the future of pharmaceutical sciences. The conference will provide an appropriate forum for participants to interact with experts, learn about emerging developments, and exchange perspectives on the evolving interface between technology and pharmaceutical research.

I am pleased to see the continued efforts of I.T.S College of Pharmacy in promoting such meaningful academic initiatives. I hope that the conference will facilitate productive discussions, create opportunities for collaboration, and leave the participants with new ideas and perspectives to carry forward in their academic and professional journeys.

I congratulate the organising committee for their efforts and convey my best wishes to all the delegates, speakers, and participants for a successful and memorable conference.

Mr. B.K. Arora
Secretary
I.T.S - The Education Group

Co-Patron's Message



In an increasingly interconnected academic and professional world, exchanging knowledge and ideas has become essential for meaningful progress. It is, therefore, with great pleasure that I extend my greetings on the occasion of the **AKTU Sponsored National Conference** being organised by I.T.S College of Pharmacy, Ghaziabad, on 11th September 2026, centred around the highly relevant theme, "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences."

Events such as this conference serve as an important meeting ground for academicians, researchers, industry professionals, and students, enabling them to connect, communicate, and engage with contemporary developments in their respective fields. The conference theme highlights the growing convergence of technology and pharmaceutical sciences and reflects the need to remain responsive to emerging trends and innovations.

I am confident that this conference will bring together diverse perspectives and create an atmosphere conducive to learning, interaction, and professional growth. It will also give young participants an opportunity to engage with experts and broaden their understanding of emerging opportunities in pharmaceutical sciences.

I commend the organising committee for conceptualising and organising this important academic event. My best wishes are with all the speakers, delegates, participants, and organisers for a successful and enriching conference.

Mr. Surinder Sood
Director - Public Relations
I.T.S - The Education Group

Guest of Honor's Message



It is a privilege to be associated with the **AKTU Sponsored National Conference** on "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences" being organised by I.T.S College of Pharmacy, Ghaziabad, on 11th September 2026.

The growing integration of technology and computational approaches into healthcare and pharmaceutical sciences holds immense promise for improving the way we understand, prevent, and manage diseases. Such interdisciplinary initiatives are essential for bridging the gap between scientific innovation and its ultimate purpose—better healthcare outcomes for society.

I appreciate the efforts of I.T.S College of Pharmacy in bringing together experts, researchers, healthcare professionals, and students on a common platform to exchange knowledge and ideas. I am confident that the deliberations during the conference will encourage meaningful discussions and inspire innovative approaches towards addressing future healthcare challenges.

I extend my best wishes to the organising committee and all the participants for a successful and intellectually enriching conference.

Wishing the conference every success.

Dr. Vimal Gupta
Director
ABYSS Pharma Pvt. Ltd., New Delhi

Guest of Honor's Message



I am pleased to extend my warm greetings to the organisers and participants of the **AKTU Sponsored National Conference** on "Computer-Aided Design Tools for Innovation in Pharmaceutical Sciences", being organised by I.T.S College of Pharmacy, Ghaziabad, on 11th September 2026.

The pharmaceutical sector is witnessing rapid advancements driven by scientific innovation, digital technologies, and evolving approaches to drug development and healthcare. In this changing landscape, the application of computer-aided tools offers significant opportunities to enhance research capabilities, support innovation, and contribute to the development of quality pharmaceutical products. The theme of this conference is both contemporary and relevant, providing an important platform for academicians, researchers, professionals, and students to deliberate on emerging developments in pharmaceutical sciences. Such scientific gatherings play a vital role in promoting knowledge exchange, encouraging collaborative research, and nurturing the next generation of pharmaceutical scientists.

I commend I.T.S College of Pharmacy for organising this important academic initiative and bringing together diverse stakeholders from academia, research, and industry. I am confident that the conference will lead to fruitful discussions and meaningful outcomes.

Wishing the conference every success.

Dr. V. Kalaiselvan
Secretary-cum-Scientific Director
Indian Pharmacopoeia Commission (IPC)
Ministry of Health & Family Welfare, Government of India

Organizing Chairman's Message



It gives me immense pleasure to welcome all the academicians, researchers, industry professionals, scholars and students to the **AKTU-Sponsored National Conference on "Computer Aided Design Tools for Innovation in Pharmaceutical Sciences."**

The pharmaceutical sciences are undergoing a remarkable transformation, driven by rapid advances in computational technologies, artificial intelligence, data analytics and digital modelling. The integration of these emerging technologies with conventional pharmaceutical research is opening new avenues for faster, smarter and more precise approaches to drug discovery, formulation development and healthcare innovation.

At I.T.S College of Pharmacy, Muradnagar, we are committed to fostering innovation, interdisciplinary learning, and meaningful research. We believe that integrating scientific knowledge with emerging technologies is essential to address the evolving challenges of pharmaceutical sciences. This conference provides a platform for sharing contemporary research, exchanging ideas, and inspiring technology-driven pharmaceutical innovation.

I am confident that the deliberations, presentations and interactions during this conference will stimulate new ideas, strengthen academic and professional networks, and contribute towards developing a culture of innovation and research.

I extend my sincere appreciation to the organizing committee, distinguished speakers, delegates, researchers, and students for their valuable contributions and active participation, which have greatly enriched the scientific deliberations and contributed to the successful conduct of this conference.

I wish the conference great success and hope that it becomes a memorable milestone in our collective journey towards innovation and excellence in pharmaceutical education and research.

Dr. S. Sadish Kumar
Director
I.T.S College of Pharmacy
Muradnagar, UP

Convener's Message



It is a matter of great privilege and enthusiasm to present the **AKTU-Sponsored National Conference on "Computer Aided Design Tools for Innovation in Pharmaceutical Sciences."**

The pharmaceutical sector is moving beyond traditional trial-and-error approaches towards data-driven, predictive and rational decision-making. Computer-aided technologies are increasingly becoming integral to areas such as molecular modelling, virtual screening, ADMET prediction, computational toxicology, formulation optimization, precision medicine and artificial intelligence-assisted drug design. These developments are redefining the way pharmaceutical problems are conceived, investigated and solved.

The present conference has been conceptualized to bring together diverse perspectives from academia, research and industry and to create an environment where emerging concepts can be discussed beyond the boundaries of individual disciplines. It aims not only to disseminate scientific knowledge but also to encourage researchers and students to critically examine how computational tools can be translated into meaningful pharmaceutical innovation.

I believe that the true strength of a scientific conference lies in the conversations it generates—the questions asked, ideas exchanged, collaborations initiated and possibilities explored. I sincerely hope that this gathering will encourage young researchers to embrace interdisciplinary approaches and develop the confidence to use modern computational tools in addressing real-world pharmaceutical challenges.

I express my heartfelt gratitude to the eminent speakers, invited experts, delegates, research scholars, faculty members, students and the organizing team for their contribution and support. Your participation adds intellectual richness and purpose to this endeavour.

May this conference inspire curiosity, foster collaboration and pave the way for innovative research in pharmaceutical sciences.

Dr. Madhu Verma
Professor
I.T.S College of Pharmacy
Muradnagar, UP

I.T.S COLLEGE OF PHARMACY

Organizes

AKTU-SPONSORED NATIONAL CONFERENCE

on

Computer Aided Design Tools for Innovation in Pharmaceutical Sciences

11th September, 2026 (Hybrid Mode)

Program Schedule

Registration (*Venue: Activity Hall*) **8:30 – 9:30 am**

INAUGURATION

Venue: Vikram Sarabhai Auditorium (2nd floor)

Arrival of Guest of Honour and Seating of Delegates in the Auditorium / Lamp Lighting	10:00-10:10 am
Welcome Address by **Dr. S. Sadish Kumar** Director, I.T.S College of Pharmacy	10:10-10:20 am
Speech by **Mr. Arpit Chadha** Vice Chairman, I.T.S-The Education Group	10:20-10:30 am
Speech by **Mr. Surinder Sood** Director-Public Relations, I.T.S-The Education Group	10:30-10:40 am
Speech by **Dr. V. Kalaiselvan** (Guest of Honor) Secretary-cum-Scientific Director Indian Pharmacopoeia Commission (IPC) Ministry of Health & Family Welfare, Government of India	10:40-10:50 am
Speech by **Dr. Vimal Gupta** (Guest of Honor) Managing Director ABYSS Pharma Pvt. Ltd.	10:50-11:00 am

SCIENTIFIC SESSIONS

SCIENTIFIC SESSION - I **DR. MOHD YASIR** **Associate Professor** **Department of Pharmacy, College of Health Sciences** **Arsi University, Asella, Ethiopia**	11:00 – 11:45 am
SCIENTIFIC SESSION - II **DR. VAISHALI M. PATIL** **Principal-Charak School of Pharmacy** **Chaudhary Charan Singh University, Meerut**	11:45 – 12:30 pm
SCIENTIFIC SESSION - III **PROF. (DR.) OZAIR ALAM** **School of Pharmaceutical Education and Research,** **Jamia Hamdard, New Delhi**	12:30 – 1:15 pm

Q & A Session	1:15 – 1:30 pm
Lunch (***Venue: Lawn Adjacent to Admin Block***)	1:30 – 2:30 pm
Oral Presentation (***Venue: R. Ahmad Hall***) &	
Poster Session [Parallel] (***Venue: Pharmacy Block – III & IV floor***)	2:30 - 3:30 pm
Award Ceremony (***Venue: Vikram Sarabhai Auditorium***)	3:30 - 4:00 pm
Closing Remarks & Vote of Thanks **(Dr. Madhu Verma, Professor)**	4:00 - 4:15 pm

Keynote Speaker – 1



Dr. Mohd Yasir
Associate Professor
Department of Pharmacy, College of Health Sciences, Arsi University, Asella, Ethiopia
mohdyasir@arsiun.edu.et

Title: Computer-Aided Formulation Designand Optimization of Advanced Drug Delivery SystemsFrom Quality by Design (QbD) to Artificial Intelligence

ABSTRACT

Developing advanced drug delivery systems increasingly requires a systematic shift from conventional trial-and-error experimentation to rational, predictive, data-driven formulation design. Quality by Design (QbD) provides a scientific framework for this transition by establishing a systematic understanding of the relationships among the Quality Target Product Profile (QTPP), Critical Quality Attributes (CQAs), Critical Material Attributes (CMAs), and Critical Process Parameters (CPPs). Within this framework, risk assessment and Design of Experiments (DoE) systematically identify and evaluate critical formulation and process variables, while statistical modeling, response surface methodology, and design-space approaches support robust optimization and deepen product and process understanding. Computer-aided formulation design further strengthens this approach by integrating experimental data with mathematical and computational models to predict formulation performance, identify optimal conditions, and reduce unnecessary experimentation. These principles are particularly relevant to advanced drug delivery systems, including nanoparticles, where critical quality attributes such as particle size, entrapment efficiency, zeta potential, and drug-release behavior strongly influence product performance and therapeutic potential. Building upon the QbD framework, the presentation will explore the emerging role of machine learning (ML) and artificial intelligence (AI) in pharmaceutical formulation development. AI-driven approaches can identify complex and nonlinear relationships among formulation variables, predict multiple quality attributes, and support rapid formulation optimization and experimental validation. Integrating QbD, DoE, and AI represents a progressive shift toward predictive, intelligent, and knowledge-driven formulation development. This integrated approach can reduce experimental burden, accelerate formulation optimization, improve product and process understanding, enhance robustness and reproducibility, and ultimately support the development of high-quality advanced drug delivery systems.

Keywords: Advanced drug delivery, Design of experiments, Optimization, Artificial intelligence, Nanotechnology.

Keynote Speaker – 2



Dr. Vaishali M. Patil,
Principal-Charak School of Pharmacy, Chaudhary Charan Singh University, Meerut
vaishalimpatil.csop@gmail.com

Title: Ligand-Based Drug Design and QSAR: From Molecular Structure to Drug Discovery

ABSTRACT

Ligand-Based Drug Design (LBDD) is a vital computational tool for rational drug discovery, especially when a high-resolution three-dimensional structure of the biological target is unavailable or ambiguous. Theknown active and inactive ligands and their experimentally determined biological activities are used to identify structural patterns associated with activity and to predict promising new compounds. The main principles, workflow, methodologies, computational tools, and applications of LBDD with particular emphasis on Quantitative Structure–Activity Relationship (QSAR) modelling were discussed. The LBDD workflow defines a reliable biological endpoint, which collects and curates molecular and activity data, selects appropriate molecular representations, calculates descriptors or fingerprints, explores structure–activity relationships, develops predictive models, and validates their performance using independent datasets. For hit identification and lead optimization, it facilitatescomplementary strategiesfor molecular similarity searching, pharmacophore modeling, QSAR, machine-learning approaches, matched molecular pair analysis, and ligand-based virtual screening. QSAR tool help to establish quantitative relationships between molecular structure-derived variables and biological activity, which utilize traditional methods such as multiple linear regression and partial least squares to machine-learning algorithms including random forest, support vector machines, gradient boosting, and neural networks. The critical considerations for best results include data quality, feature selection, prevention of data leakage, overfitting, applicability domain, chemical-space coverage, and external validation. Case studies involving COX-2, acetylcholinesterase, and BACE-1 inhibitors illustrate the practical application of ligand-based methods in drug discovery. Integration of LBDD with docking, molecular dynamics, ADMET evaluation, synthesis, and experimental testing can further strengthen decision-making. Overall, LBDD and QSAR transform available molecular activity data into actionable predictions for efficient discovery and optimization of novel therapeutic candidates.

Keywords: Ligand-Based Drug Design (LBDD); Quantitative Structure–Activity Relationship (QSAR); Molecular Descriptors; Pharmacophore Modeling; Molecular Fingerprints; Machine Learning; Virtual Screening.

Keynote Speaker – 3



Prof. (Dr.) Ozair Alam

Department of Pharmaceutical Chemistry,

School of Pharmaceutical Education and Research, Jamia Hamdard

oalam@jamiahamdard.ac.indr.ozairalam@gmail.com

Title: Target Identification to Molecule Development: Computational Strategies in the Recent Drug Discovery

ABSTRACT

In recent times, the process of drug discovery has undergone a significant transformation with the integration of computational approaches into conventional pharmaceutical research.In early-stage drug discovery, computational tools help to support in improvement of efficiency and rationality and its use extends from identification and validation of potential therapeutic targets to the development and optimization of promising drug candidates. In the session, the importance of computational tools in target identification, molecular characterization, lead identification, and structure-guided optimization is highlighted. Medicinal chemistry and molecular modelling are complementary disciplines, that enables researchers to investigate molecular structures, predict molecular interactions, explore structure–activity relationships, and prioritize compounds with desirable pharmacological properties. These can facilitate the analysis of target–ligand interactions and assist in the selection of promising molecules before extensive experimental assessment. Molecular modelling, molecular similarity analysis, pharmacophore-based approaches, quantitative structure–activity relationship (QSAR) modelling, virtual screening, and computational prediction of drug-like properties provide an integrated framework for rational molecule development. These techniques provide a basis for systematic exploration of chemical space and support the identification of structural features associated with biological activity. Importantly, the integration of computational predictions andexperimental methods is effective insynthesis, biological evaluation and refinement of predicted candidates by computational models. Such iterative integration of computational and experimental strategies can help prioritize research efforts, minimize unnecessary synthesis and biological testing, and accelerate the progression from target identification to lead optimization. Overall, computational drug discovery represents a powerful enabling strategy that complements medicinal chemistry and experimental pharmacology, contributing to more informed, efficient, and resource-conscious development of potential therapeutic agents.

Keywords: Computational Drug Discovery; Target Identification; Molecular Modelling; Medicinal Chemistry; Virtual Screening; QSAR; Pharmacophore Modeling; Structure–Activity Relationship.

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P-2	Formulation and development of phytoconstituents based herbal VapoRub
P-3	Digital Twin Technology for Pharmaceutical Product Development
P-4	Plant-Derived Bioactive Compounds as Emerging Therapeutic Leads: Molecular Docking Insights into Drug–Target Interactions
P-5	Innovations in Intranasal Nanocarrier Drug Delivery: Bridging the Gap Across the Blood–Brain Barrier
P-6	Pathophysiological Differences Between Normal And Diabetic Wound Healing
P-7	Design, Synthesis and Biological Evaluation of Novel Small Molecules Against Non-Small Cell Lung Cancer
P-8	Computational Screening of Permeation Enhancers for Enhanced Intestinal Drug Transport
P-9	In-Silico Optimization of Polymeric Nanoparticles for Superior Intestinal Permeability and Bioavailability
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Rational Design of Dual Vegfr-2 / Pparγ-Directed 5-Arylidene-Thiazolidine-2,4-Dione Hybrids Against Triple-Negative Breast Cancer An Integrated In-Silico Study

Bhavinee Sharma[1]*, Dr. Garima Kapoor[1], Prof. (Dr.) Shweta Bajaj[2]

[1]Department of Pharmaceutical Chemistry, School of pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Uttar Pradesh, India

[2]Professor and Dean, Maharishi School of Pharmaceuticals, Maharishi University, Noida campus,

bhavinee.26sphd00128@kiet.edu

ABSTRACT

Triple-negative breast cancer lacks the three receptors every targeted breast-cancer agent exploits, and no anti-angiogenic is approved for it. Thiazolidine-2,4-dione (TZD) carries one hydrogen-bond donor flanked by two acceptors — the geometry an ATP-site hinge binder requires, and the acidic head that anchors glitazones in PPARγ. Twenty-eight (Z)-5-arylidene-TZD hybrids — para-linked ureas, anilides and reverse amides plus meta-linked urea regio-isomers, each bearing one of eight terminal aryls — were enumerated with N3–H deliberately retained, embedded (ETKDGv3) and MMFF94s-minimised. Docking used AutoDock Vina 1.2.5 (exhaustiveness 16, seed 42) in focused 24 Å boxes on VEGFR-2, PPARγ and EGFR, with independent Vinardo re-docking, PLIP interaction profiling and RDKit ADMET filtering. Receptor numbering was verified at 25 landmark residues (25/25 matched), the VEGFR-2 model confirmed DFG-in/αC-in (Lys868–Glu885 salt bridge 2.98 Å), and re-docked sunitinib reproduced its hinge-bound pose. Seven hybrids scored more favourably than sorafenib at VEGFR-2 and all 28 exceeded sunitinib — best 6h (−11.52 kcal mol^{-1}), 7e (−11.37 kcal mol^{-1}), 5h (−11.32 kcal mol^{-1}). At PPARγ, 20 out-scored rosiglitazone and 7 occupied the dual-target window; 5h was nominated as lead (−11.32 and −9.87 kcal mol^{-1}). The unsubstituted core reached only −6.87 kcal mol^{-1}, confirming that affinity derives from the designed linker and tail, not the ring itself. Vina and Vinardo rankings correlated (r = 0.79). The series was PAINS-free, 26/28 met the rule of five, and synthetic accessibility (1.94–2.41) matches a two-step route. Pharmacophore-guided bioisosteric redesign of the glitazone scaffold yields synthetically simple hybrids predicted to engage both an angiogenic kinase and a differentiation-promoting nuclear receptor. These remain computational hypotheses; synthesis, VEGFR-2 kinase inhibition, PPARγ transactivation and MDA-MB-231/MCF-7 cytotoxicity assays are in progress.

Keywords: Thiazolidine-2,4-dione · VEGFR-2 · PPARγ · triple-negative breast cancer · molecular docking · bioisosterim

Formulation and development of phytoconstituents based herbal VapoRub

Smriti Sahu[1]*,

KIET Deemed-to-be-University, Ghaziabad, Delhi-NCR, Uttar Pradesh, India, 201206.

smritisahu684@gmail.com

ABSTRACT

This research article aims to formulate and evaluate herbal vaporub for the treatment of cold, mild asthma and nasal congestion. The study involves the development of formulations utilizing natural ingredients known for their analgesic and decongestant properties, such as menthol crystals, eucalyptus oil, clove oil, liquorice, ajwain and camphor. These phytoconstituents were selected due to their decongestant, anti-inflammatory, antimicrobial and bronchodilator activities. The efficacy and safety of the herbal products are evaluated through various tests, including compatibility, stability, efficacy studies, safety assessments, and optimization. The study clearly shows that a stable, patient friendly, cost-effective herbal inhaler can be formulated using natural ingredients as a potential substitute for synthetic inhalation treatments which provide valuable insights into the potential of herbal remedies for managing common respiratory ailments.

Keywords: Anti-Inflammatory, Cold, Herbal VapoRub, Nasal Decongestion.

Digital Twin Technology for Pharmaceutical Product Development

Shreya Kaushik*, Mr. Vishant Goyal

Department -Pharmacy, Samarth Institute for Education & Technology, Nek, Baghpat Road, Meerut

shreyakaushik214@gmail.com

ABSTRACT

Digital Twin (DT) technology is an emerging approach with significant potential to transform pharmaceutical product development by integrating physical systems with data-driven virtual models. A Digital Twin is a dynamic virtual representation of a product, manufacturing process, or equipment that uses experimental and process data to simulate, predict, and optimize real-world performance. By combining mathematical modeling, artificial intelligence, simulation, and real-time data, Digital Twins enable predictive and intelligent pharmaceutical innovation. The Digital Twin workflow involves systematic collection of experimental, process, and product-performance data. These data are integrated into computational models to create a virtual representation of a pharmaceutical product or process. Multiple formulation and process scenarios are simulated to predict system behavior and identify optimal conditions. The predicted outcomes are optimized and experimentally validated. This approach can support formulation optimization, process development, prediction of critical quality attributes, scale-up, and technology transfer. Digital Twin technology has considerable potential to improve pharmaceutical development. Virtual simulations can predict the influence of formulation variables and process parameters before extensive laboratory experimentation, enabling more focused and efficient studies. Digital Twins can assist in identifying optimal operating conditions and predicting critical quality attributes using real-time and historical data. They may also reduce uncertainty during scale-up and technology transfer while supporting improved quality management and evidence-based decision-making. Digital Twin technology can shift pharmaceutical development from conventional trial-and-error approaches toward predictive, connected, and data-driven innovation.

Keywords: Digital Twin; Pharmaceutical Product Development; Artificial Intelligence; Predictive Modeling; Formulation Optimization; Process Development.

Plant-Derived Bioactive Compounds as Emerging Therapeutic Leads Molecular Docking Insights into Drug–Target Interactions

Mr. Sujal*, Mrs. Khushboo Bansal

Sunder Deep Pharmacy College, SDGI Global University

sujalguru9918@gmail.com

ABSTRACT

The discovery and development of novel therapeutic agents remain major challenges in modern pharmaceutical research due to increasing drug resistance, adverse effects, high development costs, and the prolonged timeline associated with conventional drug discovery. Phytochemicals, naturally occurring bioactive constituents derived from medicinal plants, represent a valuable and structurally diverse source of potential drug candidates. Compounds such as alkaloids, flavonoids, terpenoids, phenolics, tannins, and glycosides have demonstrated diverse pharmacological activities, including antioxidant, anti-inflammatory, antimicrobial, anticancer, antidiabetic, and neuroprotective effects. However, the identification and optimization of bioactive phytochemicals through conventional experimental approaches can be laborious and time-consuming. Molecular docking has emerged as a potent computational tool for forecasting the interaction of phytochemicals with a biological target at the molecular scale. Phytochemical profiling along with molecular docking, molecular dynamics simulations, pharmacological efficiency of bioactive molecules and other computational approaches can offer a holistic understanding of the mechanisms underlying the therapeutic potential of plant-derived compounds. Computational predictions require appropriate validation through in vitro, in vivo, pharmacokinetic, toxicological, as well as clinical studies. Thus, the integration of phytochemistry and molecular docking represents a promising and futuristic approach for discovering more selective, safely and potentially effective therapeutic agents from natural bioactive compounds.

Keywords: Molecular docking, drug discovery, ligand–target, pharmacokinetic, toxicological, rational design, bioactive compounds

Innovations in Intranasal Nanocarrier Drug Delivery Bridging the Gap across the Blood–Brain Barrier

Alpana
ABESIT College of Pharmacy, Ghaziabad
alpana.alpu01@gmail.com

ABSTRACT

Nose-to-brain drug delivery has emerged as a promising strategy for enhancing the transport of therapeutic agents to the central nervous system (CNS), particularly for drugs exhibiting poor brain bioavailability and limited permeability across the blood–brain barrier (BBB). This non-invasive approach enables direct drug transport from the nasal cavity to the brain through the olfactory and trigeminal neural pathways, thereby bypassing the BBB and minimizing systemic drug exposure. Consequently, N2B delivery offers rapid onset of action while reducing peripheral adverse effects. Recent advancements in nanotechnology have significantly accelerated the development of intranasal drug delivery systems. A wide range of nanocarriers, including nanoemulsions, microemulsions, polymeric micelles, lipid-based nanoparticles, liposomes, and transfersomes, have been extensively investigated for their ability to improve drug delivery to the brain. Rapid mucociliary clearance, restricted drug-loading capacity, formulation stability, and the potential redistribution of drugs from the brain into the systemic circulation remain significant obstacles. To address these limitations, researchers are exploring innovative formulation strategies, including the incorporation of mucoadhesive polymers, surface functionalization, ligand-mediated targeting, and stimuli-responsive nanocarriers, to prolong nasal residence time and enhance drug uptake into the brain. Equally important are the safety and toxicological considerations associated with repeated intranasal administration of nanocarrier systems, highlighting the need for comprehensive preclinical evaluation and well-designed clinical studies to establish their long-term efficacy and safety.

By enabling direct, targeted, and efficient drug transport to the brain while reducing systemic exposure, this approach has the potential to overcome the limitations of conventional drug delivery systems and improve therapeutic outcomes for a wide range of neurological diseases.

Keywords: Nanostructure lipid carrier, Blood-Brain Barrier, Nanoparticles, Nanoemulsion, Liposomes, drug targeting.

Pathophysiological Differences between Normal and Diabetic Wound Healing

Raushan Kumar Singh , Dr. Snigdha Das Mandal
M.Pharm Research scholar, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
Professor, Faculty of pharmacy, Parul Institute of Pharmacy and Research, Parul University, Vadodra, Gujarat - 361760.
rks10032003@gmail.com

ABSTRACT

Wound healing is a highly regulated and complex process that involves hemostasis, inflammation, proliferation, angiogenesis, re-epithelialization and remodeling to restore tissue integrity. In diabetes mellitus this process is severely impaired by metabolic and cellular abnormalities induced by chronic hyperglycaemia. Thus, diabetic wounds are different from normal wounds and often become chronic non-healing ulcers. Peer-reviewed publications from PubMed, Scopus, and Web of Science were used in a thorough literature review. Cellular, molecular, vascular, and immunological abnormalities were highlighted in the analysis of studies comparing normal and diabetic wound healing. Normal wound healing is an ordered progression of inflammatory, proliferative and remodeling phases, which lead to timely wound closure. Conversely, diabetic wounds show prolonged inflammation due to delayed neutrophil clearance, increased pro-inflammatory cytokines and defective macrophage polarization. Diabetes causes microvascular dysfunction and impaired angiogenesis, resulting in decreased perfusion, hypoxia and decreased nutrient delivery. Fibroblast proliferation, migration and collagen synthesis are decreased leading to impaired granulation tissue formation and weak extracellular matrix deposition. Keratinocyte migration and re-epithelialization are also postponed. Moreover, oxidative stress, advanced glycation end products (AGEs) and altered growth factor signaling (e.g., VEGF; TGF-β) contribute to defective tissue remodeling and increased vulnerability to infection. Taken together, these abnormalities explain delayed wound contraction and chronic non-healing ulcers in diabetes. Diabetic wounds differ from normal wounds in persistent inflammation, impaired angiogenesis, defective fibroblast and keratinocyte function, altered extracellular matrix remodeling and increased oxidative stress. These differences in wound healing are critical to develop effective treatments to improve wound healing in diabetic condition.

Keywords: Diabetes mellitus, diabetic wound, wound healing, inflammation, angiogenesis, re-epithelialization, oxidative stress.

Design, Synthesis and Biological Evaluation of Novel Small Molecules Against Non-Small Cell Lung Cancer

Ansari Azim Zakir[1], Mohd Usman Mohd. Siddique[1], Yogeeta Agrawal[1]*
[1]Department of Pharmaceutical Chemistry, SVKM NMIMS Global University, School of Pharmacy and Technology Management, Dhule
* Department of Pharmaceutics, SVKM NMIMS Global University, School of Pharmacy and Technology Management, Dhule
azimchem313@gmail.com

ABSTRACT

Non-small cell lung cancer (NSCLC) accounts for approximately 85% of lung cancer cases and remains associated with high mortality, particularly because of late diagnosis and acquired resistance to targeted therapy. Epidermal growth factor receptor (EGFR) is an important molecular target in NSCLC; however, sequential resistance mutations such as T790M and C797S can reduce the effectiveness of earlier-generation and covalent EGFR tyrosine kinase inhibitors. The present work aims to design novel 2,4-disubstituted pyrimidine derivatives with improved activity toward resistance associated mutant EGFR while reducing affinity toward wild-type EGFR.A structure-based drug-design strategy was developed from a comprehensive literature survey. A virtual library of approximately 2000 C4-sulfonamide diversified pyrimidine analogues was generated while retaining an optimized C2 substitution. The compounds were screened sequentially against EGFR L858R/T790M (PDB 4RJ8), wild-type EGFR (4ZAU), T790M/C797S (7VRE), and L858R/T790M/C797S (8WD4). Candidate selection was based on mutant binding, wild-type-sparing tendency, favourable binding to C797S-containing EGFR, and key binding-site interactions rather than docking score alone. PHAZ138, PHAZ183, PHAZ456, PHAZ51, and PHAZ04 emerged among the leading Series-I candidates; PHAZ04 showed docking scores of -8.380 kcal/mol against 4RJ8 and -9.889 kcal/mol against 7VRE, while PHAZ138 showed -8.910 kcal/mol against the triple-mutant 8WD4 model. Representative binding-pose analysis indicated interactions within the EGFR ATP-binding region, including hinge-region and hydrophobic contacts with attention to residues Met793, Lys745, and Asp800. A 50 ns molecular-dynamics simulation of the PHAZ138 complex showed protein RMSD stabilization after approximately 10 ns, mainly around 2.4-2.9 Å, with the ligand remaining associated with the binding site despite conformational fluctuations. These computational findings support prioritization of a focused 30-40 compound experimental library for subsequent synthesis, structural characterization, and biological evaluation against mutant and wild-type EGFR/NSCLC models.

Keywords: EGFR, Non-Small Cell Lung Cancer, 2,4-Disubstituted Pyrimidines, C797S, T790M, n Molecular Docking, Molecular Dynamics, Mutant Selectivity.

Computational Screening of Permeation Enhancers for Enhanced Intestinal Drug Transport

Arpana Maurya
Department of Pharmaceutical Science
HRIT University, Ghaziabad, Uttar Pradesh 201206, India.
arpanaraj9694@gmail.com

ABSTRACT

Oral drug delivery is often limited by the low permeability of many therapeutic molecules across the intestinal epithelium, resulting in inadequate absorption and reduced systemic availability. Permeation enhancers offer a potential strategy for improving intestinal transport by temporarily modifying epithelial barriers and facilitating drug movement across the gastrointestinal membrane. Computational screening can help identify promising permeation-enhancing agents by predicting their interactions with membrane components, tight-junction proteins, transporters, and drug molecules. Molecular docking, molecular dynamics simulations, quantitative structure–activity relationship (QSAR) modelling, and molecular property prediction can be applied to examine the structural and physicochemical characteristics associated with permeation-enhancing activity. Computational analysis may also assist in evaluating factors such as membrane affinity, molecular flexibility, lipophilicity, toxicity potential, and compatibility with the therapeutic molecule. By prioritizing suitable candidates before laboratory testing, these approaches can reduce experimental screening requirements and support more rational formulation development. However, computational predictions require experimental confirmation because intestinal permeability is influenced by the complex composition of mucus, epithelial cells, enzymes, transport proteins, and physiological conditions. Integrating computational screening with in vitro and in vivo evaluation may therefore provide an efficient pathway for developing safer and more effective oral drug delivery systems. Overall, computational identification and optimization of permeation enhancers represents a promising approach for improving intestinal drug transport and enhancing the bioavailability of poorly absorbed therapeutic agents.

Keywords: Permeation Enhancers, Intestinal Drug Transport, Oral Drug Delivery, Computational Screening, Molecular Docking, Molecular Dynamics, QSAR, Intestinal Permeability, Bioavailability

In-Silico Optimization of Polymeric Nanoparticles for Superior Intestinal Permeability and Bioavailability

Arshad Saifi*
Department of Pharmaceutical Science
HRIT University, Ghaziabad, Uttar Pradesh 201206, India.
arahadsaifi30@gmail.com

ABSTRACT

Oral drug delivery is often challenged by poor solubility, gastrointestinal instability, limited intestinal permeability, and extensive first-pass metabolism, resulting in inadequate bioavailability. Polymeric nanoparticles offer a promising approach by protecting drug molecules, improving dissolution, controlling drug release, and facilitating intestinal transport. This study focuses on the **in-silico optimization of polymeric nanoparticles** using computational modelling to identify formulation characteristics associated with enhanced intestinal permeability and oral bioavailability. Key parameters such as polymer composition, particle size, surface charge, encapsulation efficiency, drug loading, and release behaviour can be systematically evaluated using computational prediction and multi-objective optimization approaches. This strategy may enable the rapid identification of optimized nanoparticle formulations, reduce experimental trial-and-error, and improve formulation development efficiency. Overall, integrating computational pharmaceutics with polymeric nanotechnology represents a promising strategy for developing effective oral nanocarriers with improved intestinal absorption and systemic drug exposure. Further **in vitro, ex vivo, and in vivo validation** is required to confirm the predicted performance and translational potential of the optimised formulations.

Keywords: In-silico optimization; Polymeric nanoparticles; Intestinal permeability; Oral bioavailability; Computational modelling; Nano-formulation.

AI and Computer-Aided Tools in Quality by Design for Pharmaceutical Formulation Design

Gorai Himadri Uttamkumar* & Dr. Puja Bhavsar

Department of Pharmaceutical Quality Assurance, Parul Institute of Pharmacy, Parul University, Vadodara-391760, Gujarat.

himadrigorai5@gmail.com

ABSTRACT

Systematic, knowledge-driven approaches are replacing traditional trial-and-error methods in pharmaceutical formulation development. Quality by Design (QbD) is to define Quality Target Product Profile (QTPP), Critical Quality Attributes (CQAs) and understand the impact of Critical Material Attributes (CMAs) and Critical Process Parameters (CPPs). Furthermore, the development is enhanced by prediction, modelling, optimisation, and data-driven decision-making using artificial intelligence (AI) and computer-aided tools. This review discusses the application of AI and computer-aided tools in pharmaceutical formulation design based on QbD. A review of the relevant scientific literature was performed to understand the role of computational approaches including Design of Experiments (DoE), multivariate data analysis, machine learning, predictive modelling and optimisation techniques. The use cases for these techniques were assessed in critical formulation variable identification, product performance and design space prediction. QbD allows for a systematic study of the relationship between formulation variables and product quality attributes with improved computer aided tools. Machine learning & AI on big data reveals hidden patterns, predicts formulation behaviour and optimises critical variables, thereby minimising number of experimental trials, development time and resource consumption. However, challenges remain, including data quality, model validation, interpretability, regulatory acceptance, and technical expertise.AI and computer aided tools are promising innovations to enhance the QbD implementation in pharmaceutical formulation design. Their inclusion can facilitate a transition from the conventional trial-and-error development to predictive, efficient and science-based formulation approaches. More research, validation and regulatory structures are necessary to enable wider adoption in pharmaceutical product development.

Keywords: Artificial Intelligence; Computer-Aided Tools; Quality by Design; Pharmaceutical Formulation Design; Machine Learning; Design of Experiments

Drug-Resistant Tuberculosis Rational Design and Development of Novel Heterocyclic Anti-Tubercular Agents

Mrunali R. Patil [1], Mohd Usman Mohd Siddique[1], Yogeeta Agrawal[2]
1. Department of Pharmaceutical Chemistry, School of Pharmacy & Technology Management, SVKM NMIMS Global University, Dhule, Maharashtra 424001, India
2.Department of Pharmaceutics, School of Pharmacy & Technology Management, SVKM NMIMS Global University, Dhule, Maharashtra 424001, India
Mrunali.Patil@svkm.ac.in

ABSTRACT

Drug-resistant tuberculosis (DR-TB), particularly multidrug-resistant tuberculosis (MDR-TB) and extensively drug-resistant tuberculosis (XDR-TB), remains a major global health challenge due to limited therapeutic options, prolonged treatment, adverse drug reactions, and emerging resistance to newer anti-tubercular agents. Although bedaquiline, pretomanid, and linezolid-based BPaL/BPaLM regimens have improved treatment outcomes and shortened therapy, their clinical utility is constrained by cardiotoxicity, hepatotoxicity, neurotoxicity, myelosuppression, and the emergence of drug resistance. These limitations highlight the need for safer and more effective anti-tubercular compounds with novel chemical scaffolds and mechanisms of action. The present research focuses on the rational design, synthesis, and biological evaluation of novel heterocyclic compounds targeting drug-resistant tuberculosis. Structure–activity relationship (SAR) analysis of existing anti-tubercular agents and literature-guided pharmacophoric requirements will be employed for scaffold selection and molecular modification. A focused library of heterocyclic derivatives will be designed using substitution pattern variation, bioisosteric replacement, incorporation of nitrogen- and sulfur-containing heterocycles, and side-chain optimization. Synthesized compounds will be characterized using melting point, TLC, FTIR, $^{1}H/^{13}C$ NMR, and mass spectrometry. In vitro antimycobacterial evaluation will include REMA, MABA, and CFU assays, along with MTT-based cytotoxicity assessment. Molecular docking, molecular dynamics simulations, and ADMET prediction will complement experimental findings and support structure–activity relationship analysis. The study aims to identify promising lead molecules with improved antimycobacterial potential and reduced toxicity, providing a rational foundation for the development of next-generation therapeutics against MDR/XDR-TB.

Keywords: Mycobacterium tuberculosis, drug-resistant tuberculosis, heterocyclic scaffolds, structure-activity relationship (SAR), molecular docking, multidrug resistance

Targeted Protein Degradation PROTACs and Molecular Glues

Sumit Yadav*
Department of Pharmaceutical Science
HRIT University, Ghaziabad, Uttar Pradesh 201206, India.
sy9151858@gmail.com

ABSTRACT

Targeted protein degradation (TPD) has emerged as an innovative approach in medicinal chemistry that removes disease-associated proteins from cells rather than simply inhibiting their biological activity. Among the most promising TPD strategies are proteolysis-targeting chimeras (PROTACs) and molecular glue degraders, which exploit the cellular ubiquitin–proteasome system to promote selective protein elimination. PROTACs are bifunctional molecules consisting of a ligand for the protein of interest, an E3 ubiquitin ligase-binding ligand, and a chemical linker that brings both proteins into proximity, facilitating ubiquitination and subsequent proteasomal degradation. In contrast, molecular glues are generally smaller compounds that induce or stabilize interactions between an E3 ligase and a target protein, resulting in its ubiquitination and degradation without requiring a conventional bifunctional structure. These approaches have expanded the range of proteins that can potentially be addressed through drug discovery, including targets that have been difficult to modulate using traditional small-molecule inhibitors. Advances in linker design, E3 ligase ligand development, structure-based drug design, chemical proteomics, and computational methods are contributing to the optimization of degrader potency, selectivity, pharmacokinetic properties, and cellular activity. Despite their potential, challenges such as molecular size, membrane permeability, oral bioavailability, tissue distribution, degradation selectivity, resistance mechanisms, and identification of suitable E3 ligases remain important considerations. Continued advances in medicinal chemistry and a deeper understanding of the cellular mechanisms governing protein degradation may enable the development of more selective and clinically useful degraders. Overall, PROTACs and molecular glues represent a significant shift from conventional occupancy-based pharmacology toward event-driven drug discovery and provide promising opportunities for developing therapies against previously challenging disease targets.

Keywords: Targeted Protein Degradation, PROTACs, Molecular Glues, E3 Ubiquitin Ligases, Ubiquitin–Proteasome System, Medicinal Chemistry, Drug Discovery, Protein Degradation

Essential Oils as Therapeutic Herbal Agents Phytochemistry and Pharmacological Activities

Tushar, Jatin, Mehul and Priyanka Bagri*

Department of Pharmacy, School of Healthcare and Allied Sciences, G.D. Goenka University, Sohna, Haryana, India.

tusharbansal278@gmail.com

ABSTRACT

Essential oils are complex; naturally occurring mixtures of volatile phytoconstituents obtained predominantly from aromatic medicinal plants and have been used traditionally as therapeutic agents for centuries. Their increasing scientific and pharmaceutical relevance is attributed to their diverse chemical composition and broad spectrum of biological activities. The phytochemical profile of essential oils is mainly characterised by monoterpenes, sesquiterpenes, oxygenated terpenoids, phenylpropanoids, and other volatile constituents, with their composition influenced by plant species, geographical origin, plant part, harvesting conditions, and extraction technique. Numerous essential oils have demonstrated promising pharmacological properties, including antimicrobial, antioxidant, anti-inflammatory, analgesic, antidiabetic, anticancer, neuroprotective, wound-healing, and hepatoprotective activities. These effects may arise from individual bioactive constituents as well as synergistic interactions among multiple components. However, considerable variation in chemical composition presents challenges for their therapeutic application, particularly with respect to reproducibility, efficacy, safety, and batch-to-batch consistency. Therefore, quality standardisation is essential for the development of essential oils as reliable herbal drugs. Modern analytical approaches such as gas chromatography–mass spectrometry (GC–MS), high-performance liquid chromatography (HPLC), chromatographic fingerprinting, and chemometric techniques are increasingly employed for authentication, identification of marker compounds, detection of adulteration, and quality assessment. This review highlights the phytochemistry, major pharmacological activities, mechanism of action, safety considerations, and current approaches to quality standardisation of essential oils, with emphasis on their potential development as evidence-based therapeutic herbal drugs.

Keywords: Essential oil, Extraction, Phytoconstituents, Pharmacological activities

Essential Oil Isolation Techniques a Comparative Evaluation of Conventional and Advanced Extraction Methods

Jatin, Tushar, Mehul and PriyankaBagri*

Department of Pharmacy, School of Healthcare and Allied Sciences, G.D. Goenka University, Sohna, Haryana, India.

jatin.gdgu2025@gmail.com

ABSTRACT

Essential oils are complex mixtures of volatile phytoconstituents that are widely investigated for their pharmacological, cosmetic, food, and industrial applications. The isolation technique employed for obtaining an essential oil plays a critical role in determining its yield, physicochemical characteristics, chemical composition, and b iological properties. Conventional approaches such as hydrodistillation, steam d istillation, hydro-distillation, and solvent-assisted techniques remain widely used because of their simplicity and accessibility. However, prolonged heating, loss of thermolabile constituents, solvent consumption, and relatively long extraction times have encouraged the development of alternative approaches. Modern techniques, including microwave-assisted extraction, ultrasound-assisted extraction, supercritical fluid extraction, solvent-free microwave extraction, and other emerging green technologies, offer potential advantages in terms of extraction efficiency, reduced processing time, lower solvent consumption, and improved preservation of volatile constituents. This article provides a comparative overview of different methods used for essential-oil isolation, with emphasis on their principles, operating conditions, extraction efficiency, advantages, limitations, and effects on the resulting chemical profile. Factors including plant material, particle size, moisture content, extraction time, temperature, pressure, and method-specific parameters are alsoconsidered. Particular attention is given to sustainable and environmentally friendly approaches that can improve recovery while minimizing degradation of bioactive constituents. A systematic understanding of these techniques can assist researchers in selecting an appropriate isolation method according to the botanical source, target constituents, and intended pharmaceutical orindustrial application.

Keywords: Essential oils; Hydrodistillation; Steam distillation; Microwave-assisted extraction; Extraction yield; GC– MS analysis; Volatile constituents

Pharma 4.0 Integration of Artificial Intelligence, Digitalization and Advanced Manufacturing Technologies in Pharmaceutical Quality Assurance

Dhrumil V. Zanzmeriya, Prof. Dr. Hiral Popaniya
School of Pharmacy, Dr. Subhash University, Gujarat, India
dhrumilzanzmeria@gmail.com

ABSTRACT

The pharmaceutical industry is currently undergoing a major transition from traditional, mostly reactive quality systems to connected, data-driven, and predictive approaches under the emerging Pharma 4.0 paradigm. Artificial intelligence (AI), digitalization, and advanced manufacturing technologies can transform pharmaceutical quality assurance (QA) by allowing real-time monitoring, predictive decision-making, better process control, and improved consistency of drug products. A targeted literature review was performed on the topics of Pharma 4.0, Quality 4.0, AI/ML, Internet of Things (IoT), digital twins, big-data analytics, Process Analytical Technology (PAT) and Real-Time Release Testing using recent scientific literature mainly published between 2023 and 2026. Relevant studies were retrieved from major scholarly databases and scientific publishers including those indexed in Scopus, Web of Science, PubMed and ScienceDirect. The literature reveals that AI and advanced analytics can enable predictive quality assessment, deviation and root cause analysis, process optimization, and early warning of quality risks. The convergence of IoT, PAT, digital twins, and continuous manufacturing provides real-time visibility of the processes and moves from end-product testing to continuous and predictive quality assurance. However, implementation is challenged by data quality and integrity, cybersecurity, system validation, regulatory uncertainty, interoperability, infrastructure requirements, and a shortage of digitally skilled quality professionals. To summarize, Pharma 4.0 has the potential to transform pharmaceutical QA from a reactive compliance function into an integrated, predictive, and risk-based quality ecosystem. Successful adoption will require not only technological integration but also strong governance, validated systems, data integrity controls, regulatory alignment, and workforce development. Further research should be directed to practical frameworks of incorporating these technologies into pharmaceutical quality management systems while maintaining GMP compliance.

Keywords: Internet of Things; Pharma 4.0; Pharmaceutical Quality Assurance; Quality 4.0; Artificial Intelligence; Digitalization; Industry 4.0; Digital Twins; Process Analytical Technology; Continuous Manufacturing.

A Review on Computational Strategies in Coumarin-Based Antimicrobial Drug Discovery ADMET Prediction and Lead Optimization

Arju1, Sucheta1*
1 Department of Pharmaceutical Chemistry, SGT College of Pharmacy, SGT University, Gurugram- 122505, Haryana, India
arjusama8@gmail.com

ABSTRACT

The increasing incidence of microbial infections and antimicrobial resistance has made it necessary to continuously discover new antimicrobial agents and effective antimicrobial agents. Coumarin, a privileged benzopyrone scaffold, has attracted great attention due to its diverse biological activities, especially antibacterial and antifungal activities. A large number of coumarin derivatives and hybrid molecules comprising pharmacologically important heterocyclic units have been investigated for their enhanced antimicrobial activity. Structured literature search was performed using PubMed, Scopus, and Google Scholar for peer-reviewed and Scopus-indexed articles. This review summarizes selected literature on coumarin-based antimicrobial drugs including structural changes, antibacterial and antifungal activities, molecular docking investigations, structure-activity correlations (SAR), and computational ADMET properties. Special attention was paid to drug-likeness, gastrointestinal absorption, lipophilicity, permeability, metabolism and toxicity parameters to understand their significance in antimicrobial lead optimization. The studied promising structure-dependent antibacterial properties of the coumarin–triazole, benzotriazole, oxadiazole, theophylline, chalcone and other heterocyclic hybrids against various bacterial and fungal strains suggest scope for further research. Molecular docking studies showed good interactions with microbial targets suggesting the possibility of these compounds as antibacterial leads. Furthermore, computational ADMET assessment demonstrated that structural alterations could significantly impact drug-likeness, absorption, permeability and toxicity profiles. Some of the prospective hybrids showed favorable drug-likeness while others showed some limitations such as low gastrointestinal absorption or anticipated toxicity. The combination of antibacterial activity, SAR analysis, molecular docking and in-silico ADMET profiling provides a powerful technique for rational evaluation and optimization of coumarin based antimicrobial medicines. Computational ADMET prediction may help early detection of pharmacokinetic and toxicological liabilities and prioritizing of attractive candidates for experimental follow-up.

Keywords: Coumarin; Antimicrobial agents; ADMET prediction; Molecular docking; Antibacterial; Antifungal; CADD.

The Future of Pharmaceutics AI-Driven Molecular Design and Nanotechnology - A Comprehensive Review

Vaghasiya Rutvi Bhaveshbhai, Dr. Payal N. Vaja
School Of Pharmacy, Dr. Subhash University, Gujarat, India
rutvivaghasiya27@gmail.com

ABSTRACT

A revolutionary paradigm change in contemporary pharmaceutics is represented by the convergence of artificial intelligence (AI) and nanotechnology. AI has become a potent instrument offering quick solutions for complex challenges in drug discovery. We present AI driven molecular design utilizing machine learning, deep learning, reinforcement learning, and generative models like GANs and variational autoencoders to accelerate de novo drug design, predict ADMET properties, optimize binding affinity, and reduce late-stage failures. Drug discovery typically costs billions of dollars and takes 10-15 years. AI drastically reduces this time by virtually screening millions of compounds, predicting protein-ligand interactions with tools like AlphaFold, and generating novel scaffolds with desired pharmacological activity.Nanotechnology offers versatile platforms such as lipid nanoparticles, polymeric micelles, solid lipid nanoparticles, dendrimers, nanoemulsions, and inorganic nano-assemblies capable of crossing physiological barriers like the blood-brain barrier, optimizing bioavailability, protecting labile drugs, and enabling targeted, controlled release. As demonstrated by COVID-19 mRNA vaccines and Doxil, nanocarriers enhance solubility and efficacy of poorly soluble BCS Class II and IV drugs while minimizing systemic toxicity.The pharmaceutical industry struggles to sustain development programs due to rising R&D costs, poor solubility of new entities, high attrition, and stringent regulations.The future lies in their synergy AI can design ideal nanoparticles by predicting optimal size, surface charge, zeta potential, drug floading, release kinetics, and in vivo stability, while nanotechnology executes precise delivery and optimizes manufacturing via Quality by Design (QbD).This review provides an overview of AI-driven molecular design coupled with nanotechnology represents not just an evolution but a complete revolution in pharmaceutics, promising safer, more effective, cost-efficient and patient-specific therapeutics.

Keywords: Artificial intelligence (AI), Molecular Design, Nanotechnology, Drug Delivery, Pharmaceutics

The Emerging Role of Ferroptosis in Parkinson's Disease Mechanistic Insights and Translational Perspectives

Narayan Kumar1, Dr. Archana Navale2
Parul University, Department of Pharmacology, Parul Institute of Pharmacy (PIP), 391760, Gujrat, India
rauneetchaudhary@gmail.com

ABSTRACT

Parkinsons disease is a condition that affects a substantia nigra in the global population. It is the condition that affects the overall functions of the brain. This disease causes the loss of neurons which causes release of the dopamine on the substantia nigra pars compacta in the brain, further progression of the disease cause death of the neurons. To ground this review in the most reliable evidence available, a thorough search was run across Scopus, PubMed, and Web of Science. Search terms were built around the most relevant concepts — 'ferroptosis AND Parkinson's disease', 'iron AND dopaminergic neurons', 'GPX4 AND neurodegeneration', and 'lipid peroxidation AND substantia nigra', among related MeSH terms. A growing and increasingly convincing body of evidence frame ferroptosis as an essential mechanism in the pathogenesis of PD. Increase in the iron within the SNpc causes lipid peroxidation due to the Fenton reaction, while the loss of GPX4 activity, decline of glutathione, and decrease in System Xc^- function all reduce the antioxidant defences of the particular neurons. NCOA4-mediated ferritinophagy further increase the labile iron pool, and neuroinflammatory microglial activation causes the ferroptotic loss of the dopaminergic neurons. This also causes the major alteration in the biochemicals like MDA, GSH, GPX4 and it also affect the ferritin level in the PD patient and in animal models. The multiple mechanisms that are interlinked with each other — including dysregulated iron homeostasis, lipid peroxidation, impaired antioxidant defence systems, mitochondrial dysfunction, abnormal p53 signalling, ferritinophagy, and neuroinflammation — Causes the ferroptotic cell death of the dopaminergic neurons. These pathogenic processes further cause progressive neuronal loss.

Keywords: Parkinson's disease, Ferroptosis, Dopaminergic neurons, Substantia nigra pars compacta, Iron homeostasis, Lipid peroxidation, Oxidative stress, Glutathione, GPX4, System Xc^-, NCOA4-mediated ferritinophagy.

Multi-Target-Directed Ligands in Alzheimer's Disease Bridging Cholinergic, Amyloid, and Tau Hypotheses

Pallavi Upadhyay1, G S Chakraborthy2
Parul University, Department of Pharmacology, Parul Institute of Pharmacy and Research (PIPR), 391760 Vadodara (Gujarat) , India
upadhyaypallavi2001@gmail.com

ABSTRACT

Alzheimer's disease is a multidimensional neurodegenerative disorder mediated by interrelated pathological cascades cholinergic deficit, amyloid-β (Aβ) aggregation, and tau excessive phosphorylation instead of a unidirectional pathway. Established monotargeted compounds (e.g., acetylcholinesterase inhibitors) offer only symptom- targeted alleviation and be unsuccessful to modulate disease propagation, emphasizing the necessity for multi-target-directed ligands (MTDLs) capable of concurrently involving cholinergic, amyloidogenic, and tau associated targets. To evaluate and validate the design of MTDLs that integrate the cholinergic, amyloid, and tau hypotheses of AD, with focus on mutual mechanistic target such as AChE's peripheral anionic binding site, GSK3β, BACE-1, and oxidative/neuroinflammatory pathways. A systematically organized literature synthesis was performed using network pharmacology and molecular docking studies, in vitro multi-mechanistic screening data (AChE/ BuChE inhibition, Aβ aggregation-inhibitory, tau kinase assays), and in vivo behavioral biochemical associations from AD models, comprising integrated pharmacophore and natural product derived MTDL classes. MTDLs integrating AChE-inhibitory and Aβ-anti-aggregation pharmacophores, or natural scaffolds (e.g., curcumin, ginkgolide derivatives), simultaneously regulate GSK3β facilitated tau phosphorylation and Nrf2/NF-κB mediated oxidative-inflammatory stress, generating synergistic neuroprotection enhanced to monotargeted agents in preclinical models. This signaling hub targeting validates a rational approach for disease-altering AD therapy, although obstacles persist in optimizing poly-pharmacological potency with blood-brain barrier permeability and target specificity. MTDLs that link the cholinergic, amyloid, and tau hypotheses indicate a potential disease-altering strategy for AD. Interlinking computational prediction with behavioral biochemical confirmation provides a clinically relevant structure for future MTDL development, especially for natural-product-derived multi-target agents.

Keywords: Alzheimer's disease; multi-target-directed ligands; cholinergic hypothesis; amyloid β; tau phosphorylation; poly-pharmacology

Non-Small Cell Lung Cancer (NSCLC)

Abhinav Pandey[1], Megha Garg[1*]
[1]School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
abhinavpandey3743@gmail.com

ABSTRACT

Non-Small Cell Lung Cancer (NSCLC) represents the primary malignancy of the respiratory system, accounting for approximately 85% of all lung cancer cases worldwide and originating within the epithelial cells of lung tissue. Characterized by uncontrolled cellular proliferation and high metastatic potential to distant organs such as the liver and brain, NSCLC poses a severe global public health challenge. According to 2022 epidemiological estimates, global cases reached 2,480,675 with 1,817,469 reported deaths, exhibiting an age-standardized rate of 23.6 per 100,000 individuals. The disease disproportionately affects men over women and exhibits significant geographic variation, with China recording the highest overall burden, followed by the United States, Japan, and India. Histologically, NSCLC is categorized into three main subtypes adenocarcinoma, squamous cell carcinoma, and large cell carcinoma. Although active and passive tobacco smoking remain the primary risk factors, non-smokers are also affected due to exposure to radon gas, ambient air pollution, occupational hazards, pre-existing pulmonary diseases, and genetic mutations. Clinical manifestations commonly include persistent cough, hemoptysis, shortness of breath, chest pain, systemic fatigue, and unexplained weight loss. Diagnostic evaluation integrates imaging modalities such as X-rays, CT scans, and alongside laboratory tests and tissue biopsies to establish precise cancer staging, ranging from localized Stage I to metastatic Stage IV. Treatment regimes are tailored to disease stage, utilizing surgical resection, radiation therapy, and systemic chemotherapy. Modern therapeutic advancements, particularly targeted molecular therapies and immunotherapies, have revolutionized clinical management by significantly improving survival outcomes and patient quality of life.

Keywords: NSCLC, LungCancer, Adenocarcinoma, Immunotherapy, Chemotherapy, Diagnosis, TargetedTherapy, Oncology

Polypharmacological Approaches Beyond Glycemic Control in Diabetes and Its Multifactorial Complications

Sana, Jagdish Kakadia
Faculty of Pharmacy, PIPR, Parul University, Waghodia, Vadodara, Gujarat, India- 391760
sanaaaa4422@gmail.com

ABSTRACT

Diabetes mellitus is a complex metabolic disorder in which persistent hyperglycemia is accompanied by insulin resistance, oxidative stress, mitochondrial dysfunction, inflammation and vascular abnormalities. These interconnected pathological processes contribute to the development and progression of diverse complications, including diabetic nephropathy, retinopathy, neuropathy and cardiovascular disease. Therefore, therapeutic strategies focused exclusively on glycemic control may not adequately address the multifactorial nature of diabetes and its complications. A literature-based review was conducted to explore emerging polypharmacological approaches in diabetes. Published evidence regarding multitarget and pleiotropic effects of antidiabetic therapies was evaluated, with emphasis on metabolic, oxidative, inflammatory, mitochondrial, renal, cardiovascular, and neurological pathways involved in diabetic complications. The reviewed evidence indicates that diabetes-associated complications arise from interconnected metabolic, oxidative, inflammatory, mitochondrial, and vascular disturbances rather than a single pathological mechanism. Polypharmacological approaches may simultaneously modulate multiple disease-relevant targets and signaling pathways, potentially providing broader therapeutic effects than conventional single-target strategies. Emerging evidence highlights the therapeutic relevance of pathways including AMPK, PI3K/Akt, NF-κB, Nrf2/ROS, and NLRP3 inflammasome signaling in regulating metabolic dysfunction, oxidative stress, inflammation, and organ injury. Multitarget agents, rational drug combinations, and drug-repurposing strategies therefore represent promising approaches for addressing the complex and interconnected mechanisms underlying diabetes and its multifactorial complications. Polypharmacology represents a promising therapeutic framework for moving beyond glycemic control toward coordinated modulation of interconnected pathways underlying diabetic complications. Future research integrating multitarget drug design, rational combinations and pathway-based approaches may help improve the prevention and management of multifactorial diabetic complications.

Keywords: Diabetes mellitus; Polypharmacology; Diabetic complications; Oxidative stress; Inflammation; Multitarget therapy; Glycemic control.

Computational Evaluation of Novel Pyrazolo[3,4-d] pyrimidin-4-one–Fused Heterocyclic Hybrids for Targeting HPV16 E6 in Cervical Cancer

Jeeva Jyothi V, Suma B V
Dept. of Pharmaceutical Chemistry, Faculty of Pharmacy, M S Ramaiah University of Applied Sciences, Bengaluru, Karnataka, India.
Jeevajyothi8890@gmail.com

ABSTRACT

Cervical cancer has been identified as one of the leading causes for cancer among women worldwide, with primary etiological factor recognised as persistent infection by high-risk Human Papillomavirus type 16 (HPV 16). The viral E6 oncoprotein targets degradation of the tumor suppressor protein p53, while the viral E7 oncoprotein binds and inactivates the retinoblastoma protein (pRb), which is ideal, highly selective therapeutic targets due to its exclusive expression in infected, malignant tissue. The present study aimed to design and computationally evaluate a focused library of novel N^1-substituted pyrazolo[3,4-d] pyrimidin-4-one hybrids incorporating quinazoline, quinoxaline, benzimidazole, benzothiazole and indazole pharmacophores as potential HPV16 E6 inhibitors. Molecular docking demonstrated favourable binding of the designed hybrids within the HPV16 E6 binding pocket, with quinazoline- and quinoxaline-based derivatives exhibiting the highest binding affinities ranging from −7.0 to −8.5 kcal/mol. Benzimidazole and Benzothiazole derivates showed additional hydrogen bonding interactions, while Indazole hybrids favours aromatic stacking interactions. Among the designed compounds, **N^1-(6,7-dimethoxyquinazolin-4-ylmethyl)-Pyrazolo[3,4-d] pyrimidin-4-one** and **N^1-(6-Fluoroquinoxalin-2-ylmethyl)-Pyrazolo[3,4-d] pyrimidin-4-one** showed best binding scores of -8.5 kcal/mol than the reference ligand, Luteolin (-8.4 kcal/mol). Interaction analysis revealed the formation of hydrogen bonds, hydrophobic interactions, and π–π interactions with key active-site residues. SwissADME prediction indicated that the majority of the compounds complied with Lipinski's rule of five and exhibited favourable drug-like and pharmacokinetic properties. A focused Library of N^1-substituted pyrazolo[3,4-d] pyrimidin-4-one hybrids incorporating Heterocyclic rings was rationaly designed for structure-based evaluation against the HPV16 E6 protein as target. The computational findings such as docking affinity, ADME properties and lipinski's rule compilation studies may identify promising lead molecules for further optimization and biological evaluation as potential therapeutics for cervical cancer.

Keywords: Pyrazolo [3,4-d] pyrimidin-4-one, Heterocyclic, HPV 16 E6 protein, Cervical cancer, Molecular docking, SwissADME, Structure-based drug design.

Advanced Drug Delivery Systems an Overview of Smart Medicine

Vaishnani Dev Ketanbhai, Professor Jay S. Upadhyay
School Of Pharmacy, Dr. Subhash University, Gujarat, India.
dp746831@gmail.com

ABSTRACT

Non-specific biodistribution, quick systemic clearance, poor water solubility, and dose-limiting toxicities are some of the major drawbacks of conventional pharmacotherapy. Smart drug delivery systems (SDDS), often known as "smart medicines," have emerged as a revolutionary paradigm in precision medicine and nanomedicine to address these challenges. These cutting-edge systems are designed to maximize local medication efficacy while greatly reducing off target side effects by autonomously modulating therapeutic release kinetics in direct response to certain physiological cues or external stimuli. In general, smart medications fall into stimulus-responsive groups that are influenced by either endogenous or external stimuli. Endogenous systems take advantage of pathological microenvironmental changes, such as dysregulated pH in endosomal compartments and tumor tissues, increased ROS concentrations, abnormal redox gradients (like intracellular glutathione), and overexpressed disease-specific enzymes (like matrix metalloproteinases). On the other hand, exogenous systems enable spatiotemporally regulated on-demand release by using carefully regulated external triggers such as near-infrared (NIR) light, alternating magnetic fields, ultrasound, and localized hyperthermia. Although there has been significant preclinical progress, clinical implementation is limited by biological obstacles such as the clearance by the reticuloendothelial system (RES), elevated interstitial fluid pressure in solid, variability in formulations, potential for immunogenic reactions, and difficulties in producing at scale in compliance with Good Manufacturing Practice (GMP) standards. Tackling these translational hurdles necessitates thorough toxicological assessment, consistent characterization standards, and the incorporation of biomimetic coatings (such as cell membrane cloaking) to enhance circulation duration. In general, sophisticated smart drug delivery systems signify an essential boundary in contemporary therapeutics, connecting nanotechnology and molecular biology to achieve genuinely individualized, targeted, and patient-specific interventions in oncology, immunology, and regenerative medicine.

Keywords: Smart Drug Delivery Systems (SDDS), Precision Medicine, Targeted Drug Delivery, Biomimetic Nanoparticles.

Development and Formulation of Anti-Hemorrhoid Alum Suppositories

Sanskruti V. Pawshe[1] and Bhavana D. Tambe

[1]*Department of Pharmaceutical Sciences and Technology, Institute of Chemical Technology, Mumbai – IndianOil Odisha Campus, Bhubaneswar, Odisha, India.*

[2]*Department of Pharmaceutical Sciences and Technology, SMBT College of Pharmacy, Nashik, Maharashtra, India.*

sanskrutipawshe2052@gmail.com

ABSTRACT

Alum is widely recognized for its astringent and hemostatic properties, yet its therapeutic use in modern dosage forms remains limited. To enhance its applicability, suppositories were developed and systematically evaluated. Alum was authenticated by ion identification tests and pH determination, ensuring purity and quality. Suppositories were prepared using the fusion method with polyethylene glycol-4000 (PEG-4000) and shea butter as bases, followed by solidification under refrigeration. The prepared formulations were assessed for physical appearance, disintegration time, in-vitro drug release, content uniformity, and weight variation. All suppositories were found to be white, odourless, bullet-shaped, smooth, and glossy with acceptable weight uniformity. Content uniformity ranged between 96–98.3%, disintegration time between 15–22 minutes, and dissolution between 80–87%. Among the three formulations, Formulation II exhibited superior performance, with shorter disintegration time (15 minutes), satisfactory dissolution (87%), and good content uniformity (96%). Thus, Formulation II was identified as the optimized formulation, offering a stable and effective alternative dosage form for Alum.

Keywords: Alum, Hemorrhoid, Rectal Suppositories, In-vitro release, Liquefaction.

Application of Quality by Design in the Development and Optimization of Pharmaceutical Formulations

Adarsh Krishna
Pharma Regulatory Affairs, Galgotias University
adarshprime108@gmail.com

ABSTRACT

Quality by Design (QbD) is a systematic and science-based approach to pharmaceutical development that emphasizes building quality into a formulation and manufacturing process from the early stages of development. Conventional formulation development often relies on trial-and-error experimentation, whereas QbD provides a structured framework for understanding the influence of formulation variables and process parameters on product quality. The present oral presentation highlights the application of QbD principles in the development and optimization of pharmaceutical formulations. The approach involves defining the Quality Target Product Profile (QTPP), identifying Critical Quality Attributes (CQAs), determining Critical Material Attributes (CMAs) and Critical Process Parameters (CPPs), followed by systematic risk assessment. Design of Experiments (DoE) and statistical optimization can be employed to investigate the effects and interactions of critical variables and establish an appropriate design space. Applications of QbD in various pharmaceutical dosage forms, including conventional, modified-release and nanotechnology-based formulations, demonstrate its potential to improve product robustness, consistency and performance while reducing development time and experimental resources. Furthermore, integration of QbD with computational and data-driven approaches offers opportunities for more efficient formulation optimization. Overall, QbD represents a proactive approach that enhances pharmaceutical product quality, supports process understanding and facilitates scientifically justified regulatory development.

Keywords: QBD, Critical Material Attributes, Design of Experiments, nanotechnology-based formulations

Repurposing Dapagliflozin as a Novel Anti-Fibrotic Strategy in the Management of Oral Submucous Fibrosis

Kunalsingh Chandel*, AnasJamsa
1.M Pharm Research scholar, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
2. Assistant Professor, Faculty of Pharmacy, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
kunalsingh_chandel@outlook.com

ABSTRACT

Oral submucous fibrosis (OSMF) is a chronic, potentially malignant disease of the oral mucosa associated with areca nut and tobacco use, characterized by transforming growth factor-beta 1 (TGF-β1)/Smad-driven fibroblast activation, myofibroblast trans-differentiation, and excessive collagen deposition. Current treatments, including hyaluronidase, corticosteroids and antioxidants, are mainly symptomatic and not disease-modifying. Dapagliflozin, a commonly used sodium-glucose cotransporter-2 (SGLT2) inhibitor for type 2 diabetes mellitus, possesses anti-fibrotic activity in cardiac, renal, and valvular tissues through mechanisms such as TGF-β1/Smadsignaling and AMPKα-dependent inhibition of fibroblast proliferation and collagen. The well-established anti-fibrotic effects of dapagliflozin aligned with the central pathogenic mechanisms of OSMF, prompting the development of a hypothesis-based drug repurposing approach. A staged translational framework was developed, beginning with an in vitro evaluation using human buccal fibroblasts stimulated with arecoline. On evaluation of expression of TGF-β1/Smadsignaling, α-smooth muscle actin and collagen I/III, a pilot randomized controlled trial would be done in patients with Stage I–II OSMF. Monitoring of tissue TGF-β1 level with the help of biomarkers will help. Burning sensation, cheek flexibility, mouth opening wills beclinical outcomes. Based on the documented pharmacological mechanisms of dapagliflozin, it might decrease myofibroblast trans differentiation and excessive collagen synthesis in OSMF through inhibition of TGF-β1/Smadsignaling and suppression of fibroblast activation via AMPKα. Thismechanistic overlap providesrationale to investigate dapagliflozin as a potential disease-modifying therapy. Dapagliflozin is a promising drug repurposing candidate for OSMF, but it has not been tested. Its established therapeutic use, oral bioavailability and mechanistically relevant anti-fibrotic effects support further pre-clinical and clinical research. If successful, the method could provide an inexpensive way to treat the underlying fibrotic process, rather than simply treating the symptoms.

Keywords: AMPKα-dependent inhibition of fibroblast proliferation and collagen, Stage I–II OSMF, TGF-β1/Smadsignaling

Repurposing Doxycycline as an Adjunctive Therapy in Type 2 Diabetes Mellitus Exploring Its Glycemic, Anti-Inflammatory and Cardiometabolic Potential

Ayush Kumar Behera[1]*, Anas Jamsa[2]
1.M. Pharm Research scholar, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
2. Assistant Professor, Faculty of Pharmacy, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
ayush.kumar.behera673@gmail.com

ABSTRACT

Type 2 diabetes mellitus (T2DM) is a progressive metabolic disorder characterized by insulin resistance, β-cell dysfunction, and chronic low-grade inflammation. Even with the availability of several potent antihyperhyperglycemic drugs, the progression of the disease and the persistence of metabolic risk still represent major therapeutic problems. A different way to find new therapeutic uses for known drugs is drug repurposing. The tetracycline antibiotic doxycycline has anti-inflammatory and matrix metalloproteinase-inhibitory properties that may provide additional metabolic benefits in type 2 diabetes. A systematic literature-based review was conducted to study the potential repurposing of doxycycline in T2DM. Pharmacologic actions, anti-inflammatory effects, glycemic outcomes, insulin sensitivity, lipid parameters and cardiometabolic effects were assessed. Recent clinical data on adjunctive treatment with doxycycline were considered conventional antidiabetic treatment Current evidence suggests adjunctive doxycycline may affect pathways of inflammation and glycemic control in patients with T2DM. A randomized controlled trial of 12 weeks duration was used to evaluate doxycycline and sitagliptin for the determination of glycemic indices, insulin sensitivity, lipid profiles, cardiometabolic risk indices and inflammatory biomarkers. Doxycycline is a good candidate for repurposing as it can target both the inflammatory and metabolic components of T2DM. More adequately powered clinical trials are needed to determine its efficacy, optimal dosage, long-term safety and therapeutic application. Future research should clarify long-term safety, cost-effectiveness, patient selection, and its optimal role in routine ulcer management.

Keywords: Type 2 diabetes mellitus, cardiometabolic risk, chronic low-grade inflammation

Computational Approaches to Precision Medicine and Personalised Drug Development

Khushi Dave, Rakesh Yadav
School of Pharmacy, National Forensic Sciences University, Gandhi nagar, Gujarat, India
khushidave27052@gmail.com

ABSTRACT

Precision medicine is transforming drug development from population-based treatment towards molecularly informed therapeutic strategies that account for inter-individual variability in disease biology and drug response. The convergence of pharmacogenomics, multi-omics, bioinformatics and artificial intelligence (AI) provides a computational framework for linking patient-specific molecular signatures with therapeutic selection, response and safety. A focused literature synthesis was undertaken to examine computational approaches spanning target identification, biomarker discovery, patient stratification, drug–target interaction prediction, virtual screening, de novo molecular design, pharmacokinetic/pharmacodynamic modelling and pharmacogenomic-guided therapy. Recent peer-reviewed literature and regulatory perspectives were critically examined to evaluate their translational relevance across the drug development continuum. Computational integration of genomic, transcriptomic, proteomic and metabolomic information enables multidimensional characterisation of disease phenotypes and identification of molecularly defined patient subgroups. Machine learning and deep learning models can support response prediction, adverse-event risk assessment, drug repurposing and lead optimisation, while network-based and structure-based approaches facilitate target prioritisation and drug–target prediction. Computational precision medicine can establish a continuous evidence framework connecting molecular profiling, predictive modelling and personalised therapeutic development. Its successful translation will depend on interoperable multi-omics datasets, explainable and reproducible models, rigorous validation and clinically meaningful biomarkers. Integrating computational intelligence with pharmacology and regulatory science therefore offers a credible pathway towards more adaptive, patient-centred and therapeutically precise drug development.

Keywords: Precision medicine; personalised drug development; pharmacogenomics; multi-omics; artificial intelligence; machine learning; computational drug discovery.

In Silico and Network Pharmacology Approaches Identify *Acacia senegal* Phytochemicals as Potential Alpha-Amylase Inhibitors

Abdulkadir Abdu
Department of Pharmaceutical Sciences, Guru Nanak Dev University, Amritsar India
gaduraabdu61@gmail.com

ABSTRACT

Diabetes mellitus is a rapidly expanding chronic disease, prompting interest in plant-derived natural products as adjuncts to conventional therapy because of its improvements in glycaemic control and reduced complications. To evaluate phytochemicals potential as α-amylase inhibitors using an integrated *in-silico* workflow. *Acacia senegal* phytochemicals retrieved from IMPPAT 2.0 database were evaluated their *in-silico* studies against α-amylase inhibitors using molecular docking, DFT, pharmacokinetic and toxicity profiling in addition to PASS prediction, network pharmacology and MD simulations. Docking of 31 compounds was carried out and the top three ligands which are; IMPHY014840 (-9.321 kcal/mol), IMPHY014838 (-9.208 kcal/mol) and IMPHY006972 (-9.026 kcal/mol) were selected. Their favorable binding energies indicated strong predicted affinity toward the selected enzyme target. DFT calculations showed identical HOMO-LUMO gaps of 6.936 eV for the first two ligands, whereas third one displayed a larger gap of 9.484 eV, indicating lower chemical reactivity. Furthermore, pharmacokinetic screening indicated high human intestinal absorption (75-86 %) and favorable Caco 2 permeability for the top three compounds, particularly for IMPHY014840 and IMPHY014838. PASS analysis suggested protease target affinity for IMPHY014840 and GPCR/transcription factor activity for IMPHY014838, expanding their therapeutic scope beyond α-amylase inhibition. MD trajectories confirmed overall complex stability, with IMPHY014838 exhibiting marginally lower ligand RMSD and therefore slightly superior dynamical stability. The present study identified IMPHY014840 and IMPHY014838 as promising α-amylase inhibitors with docking scores around -9.321 and -9.208 kcal/mol respectively. Network pharmacology further suggests that these compounds act on a broad set of diabetes related targets, supporting their value as antidiabetic lead candidates. In the combined computational evidence supports IMPHY014840 and IMPHY014838 as promising natural α-amylase inhibitors for type 2 DM management, recommending *in-vitro*, *in-vivo* and formulation optimization to address their limitations.

Keywords: *Acacia senegal,* α-amylase inhibition, molecular docking, DFT, pharmacokinetic analysis, network pharmacology, molecular dynamics.

Tripti Mishra, Dr Mamta Bishnoi.
School of Medical and Allied Science, Galgotias University Greater Noida
mishraguddi518@gmail.com

ABSTRACT

The discovery and development of novel therapeutic agents is a complex and time-consuming process that requires extensive experimental investigation. Computer-Aided Drug Design (CADD) has emerged as an important approach for accelerating drug discovery by enabling the computational analysis of molecular structures, drug–target interactions, and pharmacological properties. In recent years, the integration of Artificial Intelligence (AI) and Machine Learning (ML) has significantly enhanced the capabilities of CADD by enabling data-driven prediction, optimization, and generation of potential drug candidates. AI and ML algorithms can analyze large and complex chemical and biological datasets to support target identification, virtual screening, molecular docking, pharmacophore modeling, quantitative structure–activity relationship (QSAR) analysis, and prediction of pharmacokinetic and toxicity profiles. Deep learning approaches have further improved the prediction of molecular properties and drug–target interactions, while generative AI models offer new possibilities for de novo drug design and lead optimization. These computational approaches have the potential to reduce the time, cost, and experimental workload associated with conventional drug discovery and facilitate the identification of promising candidates at an early stage. However, the application of AI and ML in CADD also presents challenges, including limited and heterogeneous datasets, model interpretability, data quality, computational complexity, and the need for experimental validation of computational predictions. This presentation will explore the fundamental principles and applications of AI and ML in CADD, with emphasis on their role in virtual screening, molecular interaction prediction, ADMET profiling, and novel drug generation. The emerging opportunities, limitations, and future perspectives of AI-driven drug design will also be discussed, highlighting its potential to transform pharmaceutical research and accelerate the development of safer and more effective therapeutic agents.

Keywords: Artificial Intelligence, Machine Learning, Computer-Aided Drug Design, Virtual Screening, Molecular Docking, QSAR, ADMET, Generative AI, Drug Discovery.

Generative AI in Drug Discovery Designing Novel Drug Candidates Using Computer-Aided Tools

Bhawana Nath, Dr Mamta Bishnoi.
School of Medical and Allied Science, Galgotias University Greater Noida
bhawananath324@gmail.com

ABSTRACT

The discovery of novel drug candidates is a complex and resource-intensive process, traditionally involving extensive screening, synthesis, and experimental validation. The emergence of Generative Artificial Intelligence (Generative AI) has introduced a transformative approach to computer-aided drug design (CADD), enabling the computational generation of novel molecular structures with desired biological and physicochemical properties. By learning patterns from large chemical and biological datasets, generative models can explore chemical space and propose potentially promising compounds more efficiently than conventional approaches. Generative AI techniques, including variational autoencoders, generative adversarial networks, recurrent neural networks, and transformer-based models, have demonstrated potential in de novo drug design, molecular optimization, scaffold generation, and prediction of molecular properties. When integrated with established CADD approaches such as molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulations, and in silico ADMET prediction, these models can facilitate a more systematic and efficient drug discovery workflow. Such integration allows generated molecules to be evaluated and refined based on target affinity, selectivity, drug-likeness, pharmacokinetic characteristics, and potential toxicity before experimental synthesis. Despite its potential, Generative AI-driven drug discovery faces challenges related to the quality and diversity of training data, molecular validity, synthetic accessibility, model interpretability, biological relevance, and experimental validation. This presentation will discuss the principles and applications of Generative AI in CADD, emphasizing its role in de novo molecule generation and lead optimization. The integration of generative models with computational drug design strategies, current challenges, emerging applications, and future perspectives will also be explored. The convergence of Generative AI and CADD represents a promising paradigm for accelerating the identification and optimization of innovative drug candidates and advancing modern pharmaceutical research.

Keywords: Generative AI, Computer-Aided Drug Design, De Novo Drug Design, Drug Discovery, Molecular Generation, Virtual Screening, Molecular Docking, Lead Optimization.

Pharmacognostic & Phytochemical Standardization of Euphorbia neriifolia Linn. Leaves

Navneet Kaur, Vipin Saini
Department of Pharmaceutical sciences, Maharishi Markandeshwar University, Mullana, Haryana, India
manavneetkaur@gmail.com

ABSTRACT

Euphorbia neriifolia Linn. (familyEuphorbiaceae), commonly known as Indian Spurge Tree or Sehund, is a medicinally important plant traditionally used for the management of inflammation, pain, respiratory disorders, wounds, gastrointestinal ailments, and skin diseases. However, comprehensive pharmacognostic and phytochemical standards are essential to ensure the authentication, quality, and reproducibility of its leaves. The present study evaluated the pharmacognostic and phytochemical characteristics of *E. neriifolia* leaves. Macroscopic and microscopic examinations were performed to establish diagnostic anatomical features. Petroleum ether, chloroform, methanolic, and aqueous extracts were subjected to preliminary phytochemical screening, fluorescence analysis, and pH determination. Total phenolic content (TPC) and total flavonoid content (TFC) were quantitatively estimated using gallic acid and quercetin as reference standards, respectively. Macroscopic evaluation revealed simple, alternate to spirally arranged, oblong to lanceolate, thick and fleshy leaves with a characteristic milky latex. Microscopic examination demonstrated a thick epidermis, palisade and spongy mesophyll, prominent vascular bundles, anomocytic stomata, phloem fibres, spiral xylem vessels, starch grains, and unicellular uniseriate covering trichomes. The total ash, acid-insoluble ash, water-soluble ash, and sulphated ash values were 7.41 ± 0.48%, 2.69 ± 0.40%, 6.34 ± 0.38%, and 6.89 ± 0.48%, respectively, while loss on drying was 8.21%. Phytochemical screening demonstrated the presence of flavonoids, tannins, phenolic compounds, steroids, triterpenoids, carbohydrates, and saponins in different extracts. The present study establishes a comprehensive pharmacognostic and phytochemical profile of *E. neriifolia* leaves, including diagnostic morphological and anatomical characteristics, physicochemical constants, phytochemical composition, quantitative phenolic and flavonoid contents, and heavy-metal parameters.

Keywords: *Euphorbia neriifolia*; Pharmacognostic evaluation; Phytochemical screening; Standardization; Microscopy; Total phenolic content; Total flavonoid content; Heavy metals; Quality control.

AI-Driven Computer-Aided Design and Optimization of Pharmaceutical Formulations

Provat Das
Galgotias University, Gautum Budh Nagar, U.P, India
Provatdas889@gmail.com

ABSTRACT

The process of pharmaceutical formulation development is complex because it requires choosing appropriate drugs, excipients, and processing conditions that lead to formulations that are safe, effective, and stable. The conventional approach to formulation development typically requires multiple round of experiments and may, therefore, take a long time and consume many resources. Artificial intelligence and machine learning can facilitate formulation development process, as they allow to develop formula faster and more efficiently. The study presents an overview of the role of artificial intelligence and machine learning in computerized pharmaceuticals formulation development. The literature published was surveyed in order to highlight the use of formulations in modeling as well as its role in design, prediction, and optimization of formulations. The contribution of the AI-based approach to Quality by Design (QbD), Design of Experiments (DoE), the choice of drugs without excipients as well as optimization of formulation and process conditions has been analyzed. Models that utilize artificial intelligence and machine learning have shown their capacity for the prediction of many formulation characteristics important for preparation, such as release of the drug, the size of the particles, entrapment efficiency, stability, and other significant quality features. Computer-aided methods can help to find the complicated links between the preparation parameters and the product performance. By combining AI with QbD and DoE, it will be possible to minimize the number of unnecessary experiments and optimize the preparation. These methods are getting more important concerning modern delivery systems, including nanoparticles, liposomes, and drugs with controlled release. s Computer-aided design based on Artificial Intelligence seems to be a very good means to change regular development processes into predictive analysis-based ones. The usage of AI, ML, QbD, and experimental confirmation should provide more effective optimization, shorter development time, and assistance in the development of novel delivery systems. However, appropriate data and experimental confirmation will be necessary for the implementation of the process.

Keywords: Artificial Intelligence; Machine Learning; Computer-Aided Design; PharmaceuticalFormulation; Quality by Design; Formulation Optimization; Drug Delivery Systems.

Carbon Dot Based Nanodiagnostic in Pharmaceutics, Design Strategies, Diagnostic Mechanisms & Clinical Translation Challenges

Ms. Swastika Das1*, Prof. (Dr.) Mithun Bhowmick1
1Bengal College of Pharmaceutical Sciences and Research, Durgapur, 713212, West Bengal
swastikad109@gmail.com

ABSRACT

Carbon dots (CDs) are emerging carbon-based nanomaterials, generally smaller than 10 nm, that have gained increasing attention in pharmaceutical and biomedical research. Their unique optical and physicochemical properties, including strong fluorescence, high photostability, good water solubility, chemical stability, biocompatibility, low toxicity, and a high surface area-to-volume ratio, make them attractive for various applications. Their surface contains functional groups that can be easily modified to improve their performance and target specific biological molecules. These features give CDs considerable potential for nanodiagnostics, including bioimaging, biosensing, disease detection, and theranostic applications. CDs are mainly synthesized using top-down and bottom-up approaches. Top-down methods break larger carbon materials such as graphite, activated carbon, and carbon nanotubes into nanosized particles using techniques such as laser ablation, arc discharge, and chemical or electrochemical oxidation. However, some of these methods require high energy, temperature, or strong chemicals. Bottom-up methods produce CDs from small carbon sources such as citric acid, glucose, and polymers through carbonization and polymerization. Common techniques include microwave-assisted, hydrothermal, solvothermal, and thermal synthesis. Hydrothermal synthesis is widely preferred because it is simple, economical, relatively safe, and suitable for producing functionalized CDs with good optical properties. CDs can support nanodiagnosis through fluorescence, electron transfer, energy transfer, and reactive oxygen species-based mechanisms. These properties enable sensitive detection of biomolecules, pathogens, and disease-related changes. Surface functionalization and heteroatom doping can further enhance their optical properties, targeting ability, and diagnostic sensitivity. CDs can also act as drug carriers for targeted delivery and controlled release. Clinical translation of CD-based nanodiagnostics remains challenging due to concerns regarding long-term toxicity, biodistribution, reproducibility, large-scale manufacturing, standardization, and regulatory approval.

Keywords: Carbon Dots; Nanodiagnostics; Design Strategies; Diagnostic Mechanisms; Clinical Translation Challenges

The Role of Precision Medicion from Pharmacogenomics to Personalized Drug Therapy

Tisha Mangi, Dr. Snigdha Das Mandal
M pharm Pharmacology, Parul Institute of Pharmacy and Research, Parul University, Vadodra, Gujarat -361760.
Professor, Faculty of pharmacy, Parul Institute of Pharmacy and Research, Parul University, Vadodra, Gujarat - 361760.
tishamangi2002@gmail.com

ABSTRACT

Precision medicine is a modern approach that aims to provide treatment to the patients according to their individual characterics. Due to differences in the genes and other biological factors people do respond differently to the same medicine. Genomics guided treatment helps to understand how drug response, treatment effectiveness, and the risk of adverse drug reactions are affected by genetic differences. Thus, it plays a key role oin personalized drug therapy. Using review articles a literature review was carried out. The selected articles explained the development of pharmacogenetics and pharmacogenomics, the idea of precision medicine, about the personalized treatment as per the disease characteristics, genetic testing prior to treatment initiation, and the evolution of pharmaco-omics. The articles were studied and information from them was summarized to understand how precision medicine can enhance treatment while considering its benefits, challenge and its possible future potential. The reviewed literature tells us how precision medicine can help in choosing the right treatments for individual patients. Pharmacogenomic information helps to know the genetic differences that may influence drug response also helps in selecting the correct drug or dose. Pre-emptive pharmacogenomic testing can help to reduce adverse drug reactions and also helps in improving the safety and effectiveness of treatment. Precision medicine has potential use in biomarkers, disease subtyping, clinical information, and multi-omics data to identify patient groups and guide tailored treatment. However, itwidespread clinical use faces challenges such as limited evidence, differences between populations, cost, availability of testing, and the need for greater knowledge among healthcare professionals. Precision medicine is a key approch towards more personalized drug therapy. Pharmacogenomics helps to understand differences in drug response, while biomarkers and biological and clinical information can further support personalized treatment. To make precision medicine more widely useful in healthcare continued research and better clinical implementation are needed.

Keywords: Precision medicine; Pharmacogenomics; Pharmacogenetics; Personalized drug therapy; Biomarkers; Adverse drug reactions

Quality by Design-Driven Stability-Indicating Methods and Formulation Stability Assessment a Comprehensive Review

Priya Vadariya, Dr. Hiral Popaniya
School of Pharmacy, Dr. Subhash University, Gujarat, India
vadariyapriya@gmail.com

ABSTRACT

Over the last few years, the pharmaceutical industry has undergone a remarkable shift in analytical method development and formulation stability assessment with the increasing adoption of Analytical Quality by Design (AQbD). Instead of relying on conventional trial and-error approaches, AQbD follows a systematic, science- and risk-based strategy that integrates the Analytical Target Profile (ATP), risk assessment, Design of Experiments (DoE), Method Operable Design Region (MODR), and lifecycle management to develop robust, reliable, and regulatory-compliant stability-indicating analytical methods. The of the revised ICH Q2(R2) and ICH Q14 guidelines has further encouraged the development of analytical procedures based on scientific understanding, risk management, and continuous improvement throughout the method lifecycle. From 2023 to 2026, chromatographic techniques such as RP-HPLC, UHPLC, HPTLC, and LC-MS have increasingly incorporated AQbD principles to improve method robustness, impurity profiling, forced degradation studies, and overall analytical performance. At the same time, formulation stability assessment has advanced through the application of predictive stability modelling, real-time stability monitoring, green analytical chemistry, chemometric tools, multivariate statistical analysis, and artificial intelligence-assisted optimization, leading to reduced solvent consumption, shorter development time, and improved product quality. This review summarizes the recent progress in QbD-driven stability-indicating analytical methods and formulation stability assessment reported between 2023 and 2026, with emphasis on regulatory updates, analytical innovations, emerging technologies, current challenges, and future opportunities. Overall, the review highlights how integrating AQbD principles can improve analytical reliability, regulatory compliance, sustainability, and product quality throughout the pharmaceutical product lifecycle

Keywords: Analytical Quality by Design (AQbD), Stability-Indicating Methods, RP-HPLC, ICH Q14, ICH Q2(R2), Method Operable Design Region (MODR), Formulation StabilityAssessment, Design of Experiments (DoE)

Structural Insights into Molecular Biology of Metabotropic Glutamate Receptor 5

Richa P Shetty1*, Prabitha P1, Sujay Basu2, Sarvanan P3
1Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Mysuru, Karnataka, India
2Discovery Chemistry, Eurofins Advinus Discovery Services, Pvt. Ltd; Hyderabad, Telangana, India
3Department of Biotechnology and Bioinformatics, JSS Academy of Higher Education and Research, Mysuru, Karnataka, India
richashetty17@gmail.com

ABSTRACT

Metabotropic Glutamate Receptor 5 (mGluR5) represents an essential G-protein-coupled receptor (GPCR) that is one of the therapeutic receptor targets for numerous neurodegenerative disorders. The best-known lead molecule, i.e. Mavoglurant, pivots towards an allosteric binding site for Parkinson's symptomatic management. This leverages a high-resolution strategy to target diverse small molecules with molecular modelling to evaluate interactions within the 7TM helical bundle. A comparative analysis of diverse mGluR5 lead molecules at the allosteric binding pocket via RMSD MCS calculations, molecular docking studies, MMGBSA calculations, etc., including a detailed description of the mGluR1 to mGluR8 sequence alignment with further mGluR5-specific binding and mutational analysis. These were integrated with extensive pharmacophoric data with disparate site-directed mutagenesis (SDM) findings and orientation, including mGluR5 lipid membrane molecular dynamics (MD) studies. The mGluR5 consists of a bi-lobed venus flytrap domain coupled via a cysteine-rich domain to the 7TM region. Glutamate activation involves a transition from resting to active conformations, mechanistically linked via CRD movement to 7TM rotation. Multiple sequence analysis differentiates between a conserved binding motif and variable distal residues, enabling group 1 selectivity by recognising 20 unique amino acids. Subtype selectivity is achieved by extending structures, like Mavoglurant and Dipraglurant, to engage distal residues like I651, P655, Y659, N747, W758, and F788. Based on the clustering of MD configurations of time series, the structures and stabilising interactions of different lead molecules were also investigated, based on Mavoglurant output. Integrating structural biology provides a robust framework for rationalising ligand binding and predicting architecture. This effectively validates the significant role of the linker within the lead molecules as a bridge that connects the two smaller hydrophobic pockets along its mGluR5 selectivity and efficacy.

Keywords: Molecular Modelling, mGluR5, Lead Molecules, Parkinson DisorderDiscipline Pharmaceutical Chemistry

AI-Driven Drug Discovery from Virtual Screening to Precision Medicine

Aayushi Shah, Rakesh Yadav, Khushi Dave
School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat, India
aayushishah041203@gmail.com

ABSTRACT

Conventional drug discovery is a lengthy, costly and high-attrition process that requires extensive investigation from target identification to clinical development. The advancement of artificial intelligence (AI) and machine learning (ML) has introduced data-driven approaches capable of accelerating molecular screening, lead optimisation and patient stratification. The integration of these technologies across the drug discovery pipeline offers an opportunity to connect virtual screening with precision medicine, thereby supporting the development of more targeted and patient-centric therapeutic strategies. A literature-based review was conducted to examine the applications of AI across major stages of drug discovery. The reviewed approaches included virtual screening and hit identification, structure–activity relationship (SAR) modelling, de novo drug design, patient stratification and precision medicine. Deep learning and graph neural networks (GNNs) have been explored for molecular property prediction and lead optimisation, while generative models and reinforcement learning have facilitated the design of novel drug-like structures. Furthermore, AI-assisted analysis of genomic, phenotypic and real-world data has been investigated for biomarker identification, patient subgrouping and prediction of therapeutic response. The reviewed literature indicates that AI can enhance the efficiency of compound prioritisation, molecular optimisation and therapeutic decision-making by enabling the analysis of large and complex datasets. Virtual screening facilitates the rapid evaluation of extensive chemical libraries, whereas predictive and generative models support the identification and optimisation of potential drug candidates. Integration of molecular, clinical and patient-level information further enables biomarker-guided stratification and personalised treatment strategies. However, challenges involving data quality, standardisation, model interpretability, reproducibility, regulatory acceptance and ethical considerations continue to influence the translation of AI-driven approaches into clinical practice.AI-driven drug discovery represents a paradigm shift towards faster, data-driven and patient-centric therapeutic development. The integration of computational intelligence with pharmacological expertise and experimental validation can strengthen the drug discovery pipeline while supporting the objectives of precision medicine. Addressing limitations related to transparency, validation, regulation and ethics will be essential for the reliable and responsible implementation of AI in pharmaceutical and clinical research.

Keywords: Artificial Intelligence; Drug Discovery; Virtual Screening; Machine Learning; Precision Medicine; Biomarkers; De Novo Drug Design

Artificial Intelligence in ADMET Prediction and Computational ToxicologyRevolutionising Drug Discovery and Safety Assessment

Khushi Bhavsar, Anju Singhal, Khushi Dave
School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat, India
khushipbhavsar16@gmail.com

ABSTRACT

The prediction of absorption, distribution, metabolism, excretion and toxicity (ADMET) properties remains a critical challenge in drug discovery, as inadequate pharmacokinetic and toxicity profiles are major contributors to late-stage drug attrition. Conventional experimental and computational approaches are often time-consuming, resource-intensive and limited in their ability to evaluate the extensive chemical space encountered during early drug development. In this context, artificial intelligence (AI) and machine learning (ML) have emerged as promising approaches for accelerating ADMET assessment and computational toxicology. This review examines the application of contemporary AI and ML approaches in ADMET prediction and computational toxicology, with emphasis on deep neural networks, random forests, ensemble learning and graph-based models. The utility of molecular fingerprints, molecular descriptors and graph representations for predicting key pharmacokinetic and toxicity endpoints is explored. Applications involving oral bioavailability, blood–brain barrier permeability, hepatic metabolism, renal clearance and organ-specific toxicity are reviewed. Recent developments in transfer learning, multi-task learning and mechanism-informed computational toxicology are also discussed. The reviewed literature demonstrates that AI-driven models can facilitate rapid screening of large chemical libraries and provide valuable predictions of pharmacokinetic and toxicity-related properties during early drug discovery. Integration of molecular structural information with machine learning algorithms enables simultaneous evaluation of multiple ADMET endpoints. Furthermore, the incorporation of structural alerts, toxicological mechanisms and diverse biological datasets can enhance compound prioritisation and support informed decisions during lead optimisation. These approaches have the potential to reduce experimental burden and minimise the progression of compounds with unfavourable safety profiles. AI-assisted ADMET prediction and computational toxicology represent important advances towards data-driven and safety-oriented drug discovery. Despite their potential, challenges related to data quality, model interpretability, external validation and applicability domain must be addressed. Integration of AI predictions with experimental evidence, high-throughput screening and real-world data may further improve predictive reliability and facilitate safer and more efficient drug development.

Keywords: Artificial Intelligence; Machine Learning; ADMET; Computational Toxicology; Drug Discovery; Cheminformatics

De Novo Drug Designing Using Generative AI from Target Identification to Experimental Validation

Khushi Yadav, Khushi Dave
School of Pharmacy, National Forensic Sciences University, Gandhinagar, India
Khushi171002@gmail.com

ABSTRACT

Drug discovery is a complex, time-consuming and resource-intensive process that involves target identification, lead generation, optimization and extensive experimental evaluation. The emergence of **generative artificial intelligence (AI)** has introduced new possibilities in *de novo* drug designing by enabling the generation of novel molecular structures with desired structural, physicochemical and pharmacological characteristics. Integrating generative AI with established computational and experimental approaches may facilitate efficient identification and prioritization of potential drug candidates. A comprehensive literature-based review was undertaken to examine the application of generative AI across the *de novo* drug discovery pipeline. The reviewed approaches encompassed **therapeutic target identification and validation, AI-driven molecular generation, virtual screening, molecular docking, ADMET prediction, molecular dynamics simulation, synthetic accessibility assessment and experimental validation**. Different generative approaches, including deep learning and generative models, were considered with respect to their applications in molecular design and optimization. Integration with molecular docking and virtual screening enables preliminary assessment of binding interactions, while ADMET prediction supports early evaluation of pharmacokinetic and toxicity-related properties. Molecular dynamics can provide further insight into the stability of protein–ligand interactions, whereas synthetic accessibility assessment helps identify molecules with greater practical feasibility. Collectively, these complementary approaches enable progressive prioritization of promising AI-generated molecules before experimental investigation. Generative AI represents a promising advancement in *de novo* drug designing by integrating molecular generation with computational prediction and experimental validation. However, limitations related to data quality, model interpretability, molecular novelty, synthetic feasibility and prediction reliability remain. Therefore, **experimental validation is indispensable** for establishing the biological activity, safety and drug-development potential of AI-generated molecules.

Keywords: Generative Artificial Intelligence; *De Novo* Drug Design; Molecular Generation; Molecular Docking; ADMET; Molecular Dynamics; Synthetic Accessibility; Experimental Validation

Nanotechnology-Driven Innovations in Tuberculosis

Megha Garg [1,2*]

[1] School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India

[2] SRM Modinagar College of Pharmacy, Faculty of Medicine & Health Sciences, SRM Institute of Science and Technology, NCR Campus, Delhi-Meerut Road, Modinagar, Ghaziabad, 201204, Uttar Pradesh, India

meghagarg230@gmail.com

ABSTRACT

Tuberculosis (shortly TB) which is a disease caused by the bacterium Mycobacterium tuberculosis, is a serious global health issue which is prevention most affected by the emergence of drug resistance – first with the rise of multidrug-resistant (MDR) and then of extensively drug-resistant (XDR) strains. The long duration of treatment with poor tolerance due to side effects and ineffective penetration of the drug over the granulomatous lesions are the major challenges of the conventional approach for dealing with TB. Nanotechnology-based techniques are not just addressing the issues but also ushering in a new age of creativity in the spheres of targeted delivery, controlled release, and improved availability of TB drugs. The current review provides a detailed delineation of the various applications of functional nanoparticles, polymers, lipids, mesoporous silica, and carbon nanotubes for TB therapy. Additionally, it focuses on new surface modification techniques together with ligand-mediated targeting, the adaptive systems to the stimuli, and the macrophage-directed delivery strategies that are all facilitating drug accumulation in the cells and that also help penetration into the granulomas. Moreover, the nanocarrier-based strategies for squaring off against MDR/XDR-TB treatments which consist of drug co-delivery, the disabling of efflux pump, and methods to counter bacterial dormancy and latency are included in us. The review includes a of translational hurdles such as regulatory obstacles, safety concerns, toxicity, biocompatibility, and scalability, and it also recognizes the occurrence of certain trends like AI-assisted design of nanocarriers, theragnostic systems, personalized nanomedicine, and the unification of host-directed therapies.

Keywords: Tuberculosis, Nanocarriers, Drug Delivery, MDR/XDR-TB, Functionalized Nanoparticles

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Next-Generation CADD Integrating Generative AI, Multi-Omics and Molecular Dynamics for Precision Drug Discovery

Nimish Singla*[1], Navan Garg[2]
[1]Research Scholar, PCTE Group of Institutes, Ludhiana, Punjab, India, 142021
[2]Assistant Professor, PCTE Group of Institute, Ludhiana, Punjab, India, 142021
nimish.singla25@gmail.com

ABSTRACT

Advanced molecular simulations, multi-omics, structural biology, and artificial intelligence (AI) are revolutionizing the traditional paradigm of computer-aided drug design (CADD). Next-generation CADD combines these technologies to facilitate fast, more accurate, and patient-centred precision drug discovery. In this review, we have discussed the convergence of generative AI, AI-based protein structure prediction, multi-omics, including genomics, transcriptomics, proteomics, and metabolomics, and molecular dynamics (MD) simulations in contemporary CADD workflows. These three methods play complementary roles in target identification, structure-based drug design, virtual screening, de novo molecule generation, lead optimization, and early pharmacokinetic and toxicity prediction.The development of AI-based protein structure prediction provides structure prediction for previously difficult-to-characterize therapeutic targets, and generative AI for novel molecules with desirable pharmacological and physicochemical properties allows for the design and optimization of novel molecules for the discovery of drug targets. Multi-omics helps in finding disease mechanisms, molecular targets, biomarkers, and patient-specific therapeutic opportunities. MD simulations complement static docking by revealing protein flexibility and ligand-receptor interactions, conformational changes, and binding stability. These approaches can be leveraged with a data-driven model of targeting and drug discovery and patient-specific therapeutic discovery. As we have seen, the convergence of generative AI, predicted protein structure, multi-omics, and MD simulations can potentially shorten the time, cost, and attrition of conventional drug discovery and advance precision medicine. There are, however, still issues with data quality, biological validation, model interpretability, computational requirements, and regulatory acceptance. It seems that next-generation CADD is a promising way to get better at intelligent and patient-centred drug discovery.

Keywords: Computer-Aided Drug Design; Artificial Intelligence; Multi-Omics; Molecular Dynamics; Drug Discovery.

In Silico Evaluation of Phytochemical Synergy from *Aloe Vera*, *Plantago Major*, and *Calendula Officinalis* in Wound Healing

Mohit Pal[1], Ashwani Kumar[2]
Tulas Institute of Pharmacy, Tulas University, Dhoolkot, Chakrata Road, Dehradun, Uttarakhand, India - 248197
[2]Jaipur national university, Jaipur, Rajasthan-302017
Mohit.pharm@tulas.edu.in

ABSTRACT

The merging of complementary and alternative health methods with modern computational and in silico approaches allows ancient knowledge to be re-evaluated scientifically. This paradigm makes it easier to examine the bimolecular efficacy and safety of traditional therapeutic approaches, which strengthens their evidence-based use. In this way, herbal and natural therapies, which are considered cultural heritage, can be optimized using modern technologies and safely supplied to a larger population. Such a synthesis not only promotes biomedical innovation, but also ensures the preservation of centuries-old healing expertise. The current study seeks to evaluate, at the molecular level, the combined use and potential synergistic effects of Calendula officinalis, Plantago major, and Aloe vera, which have traditionally been used in wound treatment. In this context, molecular docking contacts, synergy scores, ADMET characteristics, and molecular dynamics simulations were performed on three key terpenes from C. officinalis essential oil, as well as three major alkaloids found in ethanolic extracts of P. major and A. vera. The revealed that, in addition to the high inhibitory activity of alkaloid constituents against inflammatory and microbial targets, the combination of aloe-emodin, plantamajoside, and τ-muurolol exhibited a strong molecular synergy against the T204D inflammation-related protein target. These discoveries shed light on the interactions between plant-derived chemicals and target proteins, verifying traditional applications using current scientific approaches and helping to the development of new treatment strategies.

Keywords: In-silico, medicinal plants, synergistic interaction, wound

AI and Molecular Simulation-Based Design of Smart Nanocarriers for Precision Drug Delivery

Monika[1], Priyanshu[2]
[1]BBDIT College of pharmacy, Duhai, Ghaziabad, u.p. (201206)
[2]Meerut Institute of Technology, NH-58, Partapur Bypass, Meerut. (250103)
monikaraghav1190@gmail.com

ABSTRACT

The coupling of artificial intelligence (AI) with molecular simulation underlies an evolving paradigm for the rational design of next-generation smart nanocarriers, i.e., precision drug delivery agents. In conventional nanocarrier development, the formulation variables, drug–carrier interactions as well as particle characterizations and stability and release behavior usually go through extensive experimental optimization that requires considerable time and resources. Computational approaches driven by artificial intelligence (AI) can significantly accelerate this process through prediction of key attributes of the formulation and determination of optimal combinations for drug, carrier materials and delivery parameters. Different predictions, using machine-learning and deep-learning models can be made from drug solubility to encapsulation efficiency, particle size, surface properties and cellular uptake, toxicity and even the drug-release profiles. Molecular simulation of drugs at the atomic-level, such as molecular docking, molecular dynamics (MD) simulation and quantum chemical calculations offer detailed insights into drug-polymer, drug-lipid and drug-excipient interactions., AI-based optimization can help generate stimuli-responsive nanocarriers that can trigger therapeutic agent release under the influence of certain physiological stimuli like pH, temperature, enzymes, redox conditions or disease-associated microenvironments. We can build a structure–property–formulation–performance relationship in which the molecular properties of therapeutic agents are linked upstream to the formulation and down steam performance via the nanocarrier composition. Thus, integrated approaches with AI, molecular simulation and pharmaceutical formulation science can significantly reduce the development time, experimental screening, enhance formulation prediction accuracy and progress forward towards patient-oriented drug delivery system generation. Advances in these general areas (explainable AI, multiscale simulation, digital twin, and experimental validation) while feeding back to strengthen this computational framework for precision nanomedicine.

Keywords: Artificial Intelligence; Molecular Simulation; Smart Nanocarriers; Precision Drug Delivery; Machine Learning; Molecular Dynamics; Drug–Excipient Interaction. Stimuli-Responsive Nanocarriers; Targeted Drug Delivery; Nanomedicine.

Dual Repurposing of Allopurinol and Candesartan for Alzheimer's disease an Integrated Network Pharmacology and Molecular Docking Approach

Kavinprabhu P*, Dr. Archana Navale
Department of Pharmacology, Parul Institute of Pharmacy, Parul University, Vadodara, Gujarat, India.
kavinprabhu9865@gmail.com

ABSTRACT

Alzheimer's disease (AD) is a multifactorial neurodegenerative disease characterized by oxidative stress, glutamatergic excitotoxicity, and neurovascular-neuroinflammatory dysfunction, for which there are very few disease-modifying therapies. The potential of drug repurposing is to use drugs with established safety profiles, thereby avoiding the time and cost of developing new drugs. Allopurinol is a xanthine oxidase inhibitor while candesartan is an angiotensin II receptor blocker, both of which have different mechanisms of action that are relevant to AD. To screen out the common molecular targets of both drugs Allopurinol and Candesartan for AD via network pharmacology and to further assess their binding capacity towards these targets using molecular docking. Target profiles of both allopurinol and candesartan were drawn against AD associated genes to create a drug-gene-disease interaction network. By using these shared nodes, six hub targets that were common to both drugs and AD were identified, including SRC, EGFR, PDE10A, GRIN2B, SGK1, and RET. The molecular docking of both compounds was performed with standard Vina docking against the crystal structure of these 6 targets (EGFR 1XKK; SRC 1Y57; RET 2IVS; SGK1 2R5T; PDE10A 3HQY; GRIN2B 6WHR), where the binding affinities (Vina docking scores) were reported. Common hub targets found as intersection between allopurinol, candesartan and AD pathology by network analysis were SRC, EGFR, PDE10A, GRIN2B, SGK1, and RET. The binding ability of candesartan was found to be very strong in all 6 targets (range −8.1 to −10.8 kcal/mol) in comparison with allopurinol (range −5.2 to −5.9 kcal/mol) in the docking analysis. Candesartan interacted best with PDE10A (−10.8 kcal/mol), followed by SGK1 (−9.3 kcal/mol) and RET (−8.7 kcal/mol) with candesartan, and GRIN2B (−5.8 kcal/mol) and EGFR (−5.8 kcal/mol) with allopurinol. These indicate that candesartan has a better multi-target binding profile than allopurinol, and suggest the most common targets shared by both drugs are the cyclic nucleotide signaling pathways in addition to those that involve kinase activity and glutamatergic signaling. In this integrated network pharmacology and molecular docking study, PDE10A, SGK1 and RET were selected as top targets for candesartan to be repurposed for AD and allopurinol, in lesser extent. Candesartan had a more consistent binding profile which further validated its prioritization. They could serve as a mechanistic foundation to evaluate candesartan alone or in combination with allopurinol in an in vivo preclinical model of AD.

Keywords Alzheimer's disease; Drug repurposing; Network pharmacology; Molecular docking; Allopurinol; Candesartan; PDE10A.

Unravelling the Molecular Mechanisms of Curcumin in Psoriasis Using Network Pharmacology, Molecular Docking, Molecular Dynamics Simulation, and CRISPR-Cas9–Based Target Validation

Neha Nakadi1,2, Pawan N Karwa1,2*
1Dr. D. Y. Patil Institute of Pharmaceutical Sciences and Research, Pimpri, Pune- 411018, India
2School of Pharmacy and Research, Dnyaan Prasad Global University, Pune- 411018, India
nehanakadi1004@gmail.com

ABSTRACT

Psoriasis is a chronic, immune-mediated inflammatory skin disorder characterized by persistent cutaneous inflammation, abnormal keratinocyte proliferation and differentiation, and dysregulation of multiple interconnected signalling pathways, including the IL-23/Th17/IL-17, TNF, NF-κB, and JAK/STAT axes. The complex, multifactorial nature of psoriasis highlights the need for therapeutic strategies capable of modulating multiple molecular targets simultaneously. Curcumin, a bioactive phytochemical with established anti inflammatory and antioxidant properties, has emerged as a potential candidate for targeting such interconnected pathological mechanisms; however, its molecular interactions and target-specific mechanisms in psoriasis remain incompletely characterized. Therefore, the present study employed an integrated systems-level approach combining network pharmacology, omics-based analysis, molecular docking, molecular dynamics (MD) simulation, and CRISPR-Cas9-based target validation to investigate the potential anti-psoriatic mechanisms of curcumin. Network pharmacology and target-network analysis identified several central psoriasis-associated targets, including TNF, IL6, NFKB1, AKT1, STAT3, EGFR, JUN, PTGS2, GSK3B, and MMP9. Functional enrichment analysis highlighted inflammatory and oxidative-stress-related biological processes, while IL-17, TNF, NF-κB, JAK-STAT, PI3K-Akt, and MAPK signalling pathways emerged as important molecular pathways. Molecular docking demonstrated favourable predicted interactions between curcumin and selected hub proteins, with PTGS2 showing the strongest predicted binding affinity (−8.09 kcal/mol), followed by EGFR (−7.35 kcal/mol), AKT1 (−5.58 kcal/mol), and STAT3 (−5.28 kcal/mol). Molecular dynamics simulation further supported the dynamic stability of the predicted curcumin–target complexes over 100 ns. CRISPR-Cas9-based analysis further identified predicted guide-targeting sites within the psoriasis-associated STAT3 gene on chromosome 17, providing a potential strategy for targeted functional investigation. The predicted targeting of STAT3 is biologically relevant because STAT3 is a key transcriptional regulator associated with the IL-23/Th17 axis, keratinocyte proliferation, inflammatory signalling, and psoriasis susceptibility. These findings support STAT3 as a potential molecular target for further experimental investigation and provide a framework for CRISPR-Cas9-mediated functional validation in psoriasis-relevant models.

Keywords: Curcumin; Psoriasis; Network pharmacology; CRISPR-Cas9; Molecular docking; Molecular dynamics simulation; Inflammation; Chemokine signalling

Pathophysiological Differences between Normal and Diabetic Wound Healing

Raushan Kumar Singh , Dr. Snigdha Das Mandal
M.Pharm Research scholar, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
Professor, Faculty of pharmacy, Parul Institute of Pharmacy and Research, Parul University, Vadodra, Gujarat - 361760.
rks10032003@gmail.com

ABSTRACT

Wound healing is a highly regulated and complex process that involves hemostasis, inflammation, proliferation, angiogenesis, re-epithelialization and remodeling to restore tissue integrity. In diabetes mellitus this process is severely impaired by metabolic and cellular abnormalities induced by chronic hyperglycaemia. Thus, diabetic wounds are different from normal wounds and often become chronic non-healing ulcers. Peer-reviewed publications from PubMed, Scopus, and Web of Science were used in a thorough literature review. Cellular, molecular, vascular, and immunological abnormalities were highlighted in the analysis of studies comparing normal and diabetic wound healing. Normal wound healing is an ordered progression of inflammatory, proliferative and remodeling phases, which lead to timely wound closure. Conversely, diabetic wounds show prolonged inflammation due to delayed neutrophil clearance, increased pro-inflammatory cytokines and defective macrophage polarization. Diabetes causes microvascular dysfunction and impaired angiogenesis, resulting in decreased perfusion, hypoxia and decreased nutrient delivery. Fibroblast proliferation, migration and collagen synthesis are decreased leading to impaired granulation tissue formation and weak extracellular matrix deposition. Keratinocyte migration and re-epithelialization are also postponed. Moreover, oxidative stress, advanced glycation end products (AGEs) and altered growth factor signaling (e.g., VEGF; TGF-β) contribute to defective tissue remodeling and increased vulnerability to infection. Taken together, these abnormalities explain delayed wound contraction and chronic non-healing ulcers in diabetes. Diabetic wounds differ from normal wounds in persistent inflammation, impaired angiogenesis, defective fibroblast and keratinocyte function, altered extracellular matrix remodeling and increased oxidative stress. These differences in wound healing are critical to develop effective treatments to improve wound healing in diabetic condition.

Keywords: Diabetes mellitus, diabetic wound, wound healing, inflammation, angiogenesis, re-epithelialization, oxidative stress.

Network Pharmacology in Computer Aided Drug Discovery for Rheumatoid Arthritis Current Evidence on Multitarget Phytochemicals

Mohd Ibrahim Sisodia*, Dr. Kinjal Bera
Department Of Pharmacology, Parul Institute of Pharmacy, Parul University, Vadodara, Gujrat, India
2508212220006@paruluniversity.ac.in

ABSTRACT

Rheumatoid arthritis (RA) is an autoimmune condition, where multiple inflammatory and tissue-destructive pathways are simultaneously active. This biological complexity can hinder the effectiveness of therapies that target only one target in the long run. Many natural compounds have multiple protein targets and signalling pathways, which suggests that they may provide a more comprehensive treatment option. It explores the mechanism of multiple targets of phytochemicals investigated in RA and the role of network pharmacology in understanding and prioritizing these targets. A narrative review of published literature was conducted to gather evidence related to pathogenesis of RA, inflammatory biomarkers, intracellular signalling pathways, medicinal plants and network pharmacology-based drug discovery. Reported compound-target associations, protein-protein interaction networks, pathway enrichment and available experimental data were focused on. The evidence reviewed indicates that closely related pathways are involved in the perpetuation of RA progression, such as NF-κB, JAK/STAT, MAPK, PI3K/Akt/mTOR, NLRP3, HIF-1α and Nrf2/HO-1. Several phytochemicals have been studied extensively, such as curcumin, quercetin, berberine, resveratrol, sinomenine, triptolide, celastrol and paeoniflorin, and have been associated with more than one inflammatory/tissue-remodelling target. The published network studies indicate that these compounds can act together to affect the release of cytokines, oxidative stress, activation of synovial fibroblasts, angiogenesis, osteoclast formation and the Th17/Treg imbalance. However, the are different depending on the quality of the database, the target-prediction approach and the extent of experimental verification. Network pharmacology offers a practical approach to structure the existing evidence and to gain insight into plant-derived compounds potential action in the complex biology of RA. Predictions should be regarded as hypothesis rather than proof of effectiveness. The future research needs to integrate computational with pharmacokinetics, standardized laboratory validation, multi-omics analysis and biomarker-related research.

Keywords: Rheumatoid arthritis; Network pharmacology; Phytochemicals; Multitarget therapy; Computer-aided drug discovery

Rheumatoid Arthritis Pharmacotherapy Current Strategies and Emerging Targeted Therapies

Sweta C. Pandey*, Jainee Vashi
Department of Pharmacology, Parul Institute of Pharmacy and Research, Faculty of Pharmacy, Parul University, Vadodara, Gujarat, India.
swetapandey28092000@gmail.com

ABSTRACT

Rheumatoid arthritis (RA) is a chronic autoimmune inflammatory disorder causing progressive synovial inflammation, joint destruction, disability, and systemic complications. Pharmacological management aims to achieve sustained remission, prevent structural damage, and improve quality of life. To provide an overview of contemporary pharmacological strategies in RA, emphasizing disease-modifying antirheumatic drugs (DMARDs), targeted therapies, and individualized treatment. A narrative review of established and emerging pharmacological approaches was undertaken, focusing on conventional synthetic DMARDs, biologic DMARDs, targeted synthetic DMARDs, glucocorticoids, and non-steroidal anti-inflammatory drugs. Methotrexate remains the preferred initial conventional synthetic DMARD, with hydroxychloroquine, sulfasalazine, and leflunomide used according to disease severity and patient factors. Patients with inadequate response may require biologic agents targeting TNF-α, IL-6, CD20, or T-cell co-stimulation, or targeted synthetic DMARDs such as Janus kinase (JAK) inhibitors. Short-term glucocorticoids may provide rapid symptom control but require cautious use because of cumulative adverse effects. Treatment selection should incorporate disease activity, comorbidities, infection risk, treatment safety, and patient preferences. A treat-to-target, individualized pharmacological approach with early DMARD initiation and regular disease-activity assessment is central to improving RA outcomes. Advances in targeted therapies continue to expand therapeutic options while emphasizing the importance of safety monitoring and rational treatment selection.

Keywords: Rheumatoid arthritis; Pharmacotherapy; Disease-modifying antirheumatic drugs (DMARDs); Methotrexate; Biologic DMARDs; JAK inhibitors; Targeted synthetic DMARDs; Treat-to-target; Immunomodulation; Precision medicine.

Therapeutic Insights into the Antidiabetic Activity of Selected *Annona* Species a Comprehensive Review

Manali Chaudhari*, Jagruti Patil, M. B. Gagarani, I. E. Ansari
Department of Pharmacology, R. C. Patel Institute of Pharmaceutical Education and Research, Shirpur, Dhule, Maharashtra, India-425405
chaudharimanali1804@gmail.com

ABSTRACT

Several tropical fruit-bearing plants with a long history of medical use belong to the *Annona* genus. Biologically active substances including alkaloids, flavonoids, tannins, and acetogenins, which are abundant in these plants, have drawn interest in recent studies due to their potential as treatments, especially for the treatment of diabetes and other metabolic diseases. *Annona squamosa* (sweetsop), *Annona muricata* (soursop), *Annona reticulata* (custard apple), and *Annona cherimola*(cherimoya) are the four *Annona* species whose antidiabetic qualities are the focus of this review. These species' bioactive compounds have a variety of pharmacological effects, including as insulin like activity, hypoglycemic effects, inhibition of enzymes that hydrolyse carbohydrates, modulation of lipid metabolism, and stimulation of glucose absorption. According to data from both in vitro and in vivo research, these plants may help improve insulin sensitivity, lower blood glucose levels, and lessen the consequences of diabetes. Their potent anti-inflammatory and antioxidant properties provide further advantages by shielding pancreatic β-cells and preventing oxidative stress, which is a major factor in the development of diabetes. Furthermore, changes in lipid profiles show how effective they are at treating dyslipidaemia associated with diabetes. In , the varied phytochemical components of the investigated *Annona* species indicate great promise as natural antidiabetic medicines. Preclinical evidence is encouraging, but before they can be suggested for routine clinical usage, thorough clinical studies are needed to determine their therapeutic effectiveness and safety in human patients.

Keywords: Diabetes mellitus, *Annona* species, Preclinical studies, In-vitro studies, Herbal drugs, Antidiabetic activity

From Molecules to Medicines Leveraging Computer-Aided Drug Design for Innovation in Pharmaceutical Chemistry

Ms. Dnyaneshwari B. Sapkal
Department of Pharmaceutical Chemistry, Bombay Institute of Pharmacy & Research, Dombivli, Maharashtra, India
dnyaneshwari165@gmail.com

ABSTRACT

The process of identifying and developing new therapeutic agents is difficult and time-consuming, involving a methodical assessment of molecular characteristics, biological activity, and drug-likeness. By offering effective computer-aided drug design (CADD) techniques for the identification and optimization of possible therapeutic candidates, recent developments in computational science have revolutionized pharmaceutical chemistry. Early-stage drug development can be accelerated while experimental costs and time are decreased by integrating computational techniques with traditional pharmaceutical research. The implementation of computational techniques such as molecular docking, molecular dynamics simulation, virtual screening, pharmacophore modeling, quantitative structure–activity relationship (QSAR) analysis, and in-silico ADMET prediction is highlighted in this work. These methods can be used to analyze key pharmacokinetic and toxicity characteristics, predict binding affinity, assess structural requirements for biological activity, and examine ligand–target interactions. Additional support for hit discovery, lead optimization, and logical chemical structure alteration can be provided via computational platforms and databases. Molecular interactions, binding patterns, physicochemical qualities, drug-likeness, and ADMET features can all be learned through the integration of CADD techniques. These computational insights can help researchers reduce the number of compounds that need to be screened experimentally and prioritize promising molecules for further laboratory study. Computer-aided methodologies are a significant advancement in pharmaceutical chemistry and provide a logical, economical, and timely approach to contemporary drug development. The drug discovery process can be strengthened and safer and more promising therapeutic options can be found more easily by combining computational predictions with experimental validation.

Keywords: Computer-Aided Drug Design, Pharmaceutical Chemistry, Molecular Docking, Virtual Screening, QSAR, ADMET, Drug Discovery

Integrative Network Pharmacology and Multi-Omics Analysis Reveals Potential Therapeutic Targets and Molecular Mechanisms of Caffeic Acid Phenethyl Ester (CAPE) in Breast Cancer

Pawan N Karwa[1,2], Nikhil S Sakle[3], Harshad S Kapare[1,2*]
1.Dr. D. Y. Patil Institute of Pharmaceutical Sciences and Research, Pimpri, Pune- 411018, India
2. School of Pharmacy and Research, Dnyaan Prasad Global University, Pune- 411018, India
3. Y. B. Chavan College of Pharmacy, Dr. Rafiq Zakaria Campus, ChhSambhajinagar, Maharashtra, 431001, India
karwapawan99@gmail.com

ABSTRACT

Breast cancer is one of the most commonly diagnosed malignancies worldwide and remains a major cause of cancer-related morbidity and mortality. Despite advances in treatment, tumor heterogeneity, therapeutic resistance, recurrence, and treatment-associated adverse effects remain major challenges. Caffeic acid phenethyl ester (CAPE), a bioactive phenolic compound derived from propolis, possesses anticancer, anti-inflammatory, antioxidant, and antiproliferative properties; however, its molecular mechanisms in breast cancer remain incompletely understood. An integrated network pharmacology and multi-omics framework was employed, incorporating protein–protein interaction (PPI), compound–target–pathway network, Gene Ontology (GO) and KEGG enrichment, gene-expression, correlation, survival, protein/oncoprotein, molecular docking, and molecular dynamics (MD) analyses. PPI analysis identified ESR, PIK3CA, EGFR, MAPK1, and PGR as key targets, while omics analysis highlighted AR, MDM2, and IGF1R. Pathway enrichment implicated the PI3K/Akt, estrogenic receptor, and apoptosis-related pathways. AR and IGF1R showed higher expression in tumour samples, whereas MDM2 exhibited comparable expression between groups. Docking demonstrated favourable CAPE binding to AR (−7.4 kcal/mol), MDM2 (−6.0 kcal/mol), and IGF1R (−5.2 kcal/mol). Among five prioritized targets, CAPE showed the strongest predicted binding to ESR (−6.12 kcal/mol). The ESR–CAPE complex remained stable during 100-ns MD simulation, exhibiting a mean backbone RMSD of 2.84 Å and favorable MM-GBSA binding free energy of −27.67 kcal/mol, with interactions involving Leu525 and Trp383. AR and IGF1R demonstrated a strong positive correlation ($r = 0.49$, $p < 0.001$), while AR–MDM2 and MDM2–IGF1R showed weak negative correlations. None of the three genes showed significant associations with overall survival. Oncoprotein analysis revealed alterations in AR (13%), MDM2 (<1%), and IGF1R (1%), with an overall alteration frequency of 14% across 2694 samples. CAPE may exert potential anti-breast cancer effects through multi-target and multi-pathway mechanisms. The integrated findings identify ESR, AR, and IGF1R as promising molecular targets and provide a mechanistic basis for further experimental validation of CAPE as a potential therapeutic candidate for breast cancer.

Keywords: Caffeic acid phenethyl ester (CAPE); Breast cancer; Network pharmacology; Multi-omics; Gene expression survival analysis; Molecular docking; Molecular dynamics simulation

Corticosteroid Resistance in Asthma a Unified Systems-Level Mechanistic Framework and Translational Perspectives

Sujay Shukla *, Dr. Ajay B. Shelke
Department of Pharmacology, Parul Institute of Pharmacy, Parul University, Vadodara, Gujarat
shuklasujay2003@gmail.com

ABSTRACT

Asthma is a common disease with more than 260 million sufferers globally and continues to be an important cause of morbidity and mortality from respiratory diseases. Despite the importance of corticosteroids as the first-line drugs for the management of asthma, up to 5-10% of patients suffer from steroid resistance. There is increasing recognition that steroid resistance involves multiple interactions between molecular pathways.Literature search through PubMed, Embase, and Web of Science databases from 1994 to 2024 with **Keywords** "corticosteroid resistance," "glucocorticoid resistance," "severe asthma," "HDAC2," "PI3Kδ," "Th17,"In this, we have compiled the current literature on steroid resistance in five inter-related regulatory pathways oxidative stress, epigenetic remodeling, immune endotype switching, cell signaling, and GR malfunction.The PI3Kδ signaling is upregulated due to oxidative stress, which causes inactivation of HDAC2 and decreased transrepression of glucocorticoids, while SIRT1 downregulation in further epigenetic defects. Th17 and ILC3-driven neutrophilia can be induced due to these changes and is accompanied by excessive GRβ expression and GRα signaling impairment. This complex of interactions forms a positive feedback system for corticosteroid resistance. Corticosteroid resistance is the result of failure at the systems level due to interconnecting regulatory networks. Therapeutic approaches involving the PI3Kδ-HDAC2-SIRT1 pathway along with immune endotype-related and receptor-related aberrations, based on omics-based biomarkers, could pave the way for precision medicine in the future.

Keywords: Corticosteroid resistance; asthma; oxidative stress; HDAC2; epigenetics; PI3K; glucocorticoid receptor; Th17; precision medicine

Computer-Aided Selection of Pharmaceutical Excipients a Smart Approach to Formulation Development

SuyashTomar*, Dr. Nidhi Namdev
GRY Institute of Pharmacy, Borawan, District Khargone, MP.
suyasht1702@gmail.com

ABSTRACT

Pharmaceutical excipients play a vital role in determining the quality, stability, manufacturability, and therapeutic performance of pharmaceutical dosage forms. However, conventional excipient selection often depends on trial-and-error experimentation, literature surveys, and formulators' experience, making formulation development time-consuming and resource-intensive. With advances in computational technologies, computer-aided approaches are emerging as smart tools for the rational selection and optimization of pharmaceutical excipients. Computer-aided excipient selection integrates formulation databases, physicochemical property prediction, molecular modeling, in-silico compatibility assessment, artificial intelligence (AI), machine learning (ML), and statistical tools to support informed formulation decisions. These approaches can predict potential drug–excipient interactions, assess compatibility, identify suitable functional excipients, and optimize formulation variables before extensive laboratory experimentation. Computational tools can also facilitate the development of immediate-release, sustained-release, and targeted dosage forms by predicting the influence of excipients on drug release, solubility, stability, and manufacturability. Furthermore, integration of these technologies with Quality by Design (QbD) and Design of Experiments (DoE) provides a systematic approach for establishing relationships between excipient properties, formulation variables, and critical quality attributes. This strategy can reduce experimental workload, material consumption, development time, and overall cost while improving formulation robustness and reproducibility. Although challenges related to data availability, model validation, and regulatory acceptance remain, the integration of artificial intelligence and computational modeling has significant potential to transform traditional trial-and-error formulation development into a faster, predictive, and scientifically rational process. Thus, computer- aided excipient selection represents a promising approach for accelerating the development of safe, effective, and high-quality pharmaceutical products.

Keywords: Pharmaceutical excipients; Artificial intelligence; Machine learning; Drug–excipient compatibility; QbD, etc.

AI-Enhanced Virtual Screening in Computer-Aided Drug Discovery

Niyati Pujari, Khushi Dave
School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat, India
niyatipujari2004@gmail.com

ABSTRACT

Conventional drug discovery is a resource-intensive and high-attrition process, often requiring extensive time and financial investment to identify viable therapeutic candidates. Virtual screening (VS) represents a fundamental component of computer-aided drug discovery (CADD), enabling the rapid in silico evaluation of large chemical libraries against defined biological targets. However, conventional approaches, including molecular docking and pharmacophore modelling, may be constrained by limitations in scoring accuracy, false-positive predictions and computational scalability, particularly when applied to ultra-large chemical libraries. These limitations have accelerated the integration of artificial intelligence (AI) into virtual screening workflows. A literature-based review was undertaken to evaluate contemporary machine learning (ML) and deep learning (DL) methodologies applied to AI-enhanced virtual screening. The review encompasses graph neural networks (GNNs), convolutional neural networks (CNNs) and generative models used in structure-based and ligand-based screening, as well as deep learning-assisted docking refinement, AI-driven quantitative structure–activity relationship (QSAR) modelling and generative scaffold design. Their applications in molecular recognition, hit identification and lead optimisation were critically examined. The reviewed literature indicates that AI-enhanced virtual screening can improve the prioritisation of potential hits by integrating complex molecular and biological features into predictive models. GNNs and CNNs facilitate the analysis of molecular structures and protein–ligand interactions, while AI-assisted docking and QSAR models enhance the prediction of binding-related properties. Generative approaches further expand chemical space by supporting the design of novel scaffolds and optimisation of promising leads. These integrated strategies demonstrate potential for improving screening efficiency, hit prioritisation and scalability across large chemical libraries while reducing computational burden. AI-enhanced virtual screening is transforming the CADD landscape by integrating computational intelligence with conventional molecular modelling approaches. Despite its considerable potential, challenges associated with data quality, model interpretability, external validation and generalisability across diverse targets remain. Future integration of AI-based screening with experimental validation and multidisciplinary drug discovery workflows may further enhance the reliability, scalability and translational utility of virtual screening.

Keywords: Artificial Intelligence; Virtual Screening; Computer-Aided Drug Discovery; Machine Learning; Deep Learning; Molecular Docking; QSAR

The Clinical Evolution of Non-Invasive Aesthetic Dermatology

1. Nibir Ghosh *, 2. Debasish Biswas
1. Assistant Professor, Department of Pharmacology, Eminent College of Pharmaceutical Technology, Kolkata
2. MBBS, MD, Dermatology, Founder and Owner Radiant Aesthetics, Kolkata
nibir@ecpt.in

ABSTRACT

Noninvasive aesthetic cosmetology has emerged as a transformative approach in the domain of dermatological sciences, providing effective alternatives to traditional invasive procedures. With advances in technology and patient-centered care, noninvasive modalities such as chemical peels, microdermabrasion, laser therapies, radiofrequency, ultrasound-based devices, and injectable treatments have demonstrated significant efficacy in managing a variety of cutaneous concerns, including photoaging, acne scars, hyperpigmentation, and skin laxity. These interventions are designed to enhance skin quality, improve patient satisfaction, and minimize recovery time, thereby offering an improved therapeutic profile compared to surgical methods. The increasing popularity of noninvasive aesthetic techniques is driven by their safety, cost-effectiveness, and ability to cater to diverse skin types and patient preferences. Moreover, their role extends beyond cosmetic enhancement, as they contribute to psychological well-being and self-esteem, factors that are increasingly recognized as integral to holistic dermatological care. Recent research highlights how combining multiple noninvasive techniques yields synergistic outcomes, further expanding their scope in clinical practice. This work aims to explore the scientific and clinical impact of noninvasive aesthetic cosmetology within dermatology, emphasizing innovations, therapeutic benefits, and future directions. By bridging cosmetic demands with evidence-based dermatological practice, noninvasive cosmetology is redefining patient care standards and shaping the future of skin health.

Keywords: Dermatology, Aesthetic, Non-Invasive, cosmetic, etc.

Emerging Herbal Therapeutics for Hemorrhoids from Traditional Medicine to Evidence-Based Clinical Practice

Piyush Jain, Snigdha Das Mandal
[1]M Pharm Research scholar, Parul Institute of Pharmacy and Research, Parul University, Vadodara, Gujrat 391760
[1]Professor, Parul Institute of Pharmacy and Research, Parul University Vadodara Gujrat 391760
jainp0340@gmail.com

ABSTRACT

Hemorrhoids are one of the most frequent pathological conditions that affect the anorectal region of millions of people worldwide, significantly decreasing their quality of life. Among the most common symptoms are pain, bleeding, itching, swelling, and tissue prolapse. Topical glucocorticoids, analgesics, and surgery have been reported as efficacious but may be associated with adverse effects, recurrence, and post-operative discomfort. Therefore, alternative herbal treatment options are of interest for the management of the disease. The purpose of this review is to present and discuss recent advancements in hemorrhoids treatment using herbal medicine. The efficacy, mechanism of action, safety, and future prospects of herbal treatment were evaluated and analyzed. A comprehensive search of PubMed, Scopus, Google Scholar, and Web of Science databases was performed to identify relevant preclinical and clinical studies published in 2015-2026. The inclusion criteria comprised articles focusing on herbal treatment of hemorrhoids in vivo and in vitro, evaluating the pharmacological potential and efficacy of herbal medicine, assessing the safety profile of phytochemicals, and investigating novel dosage forms and routes of drug delivery. The bibliographic database was screened for case reports, clinical studies, reviews, and commentaries. The review provides experimental and clinical evidence for the beneficial effects of Aloe vera, Aesculus hippocastanum, Hamamelis virginica, Azadirachta indica, Curcuma longa, and flavonoides in hemorrhoid treatment. The anti-inflammatory, antioxidant, anti-venomous, analgesic, antimicrobial, and healing properties of herbal preparations were reported. Moreover, the novel generation of herbal medicines including gels, creams, and nanoparticle formulations showed enhanced bioavailability, targeted action, and reduced side effects. Particular attention was drawn to the promising synergy of standardized herbal preparations and conventional medical care. Herbal medicine presents an effective and innovative approach to hemorrhoid treatment and management. The continuous development of phytomedicine, including the novel dosage forms and nanotechnology applications, has increased the confidence in herbal treatment. Further clinical studies and quality assurance analyses are required for the complete integration of herbal medicine into modern healthcare systems for the best patient outcome.

Keywords: Hemorrhoids; Herbal therapeutics; Phytomedicine; Traditional medicine; Evidence-based medicine; Herbal gel; Clinical practice; Drug delivery.

Multi-Omics-Guided Computer-Aided Drug Design for Precision Oncology

Komal Rani*, Navan Garg
Research Scholar, PCTE Group of Institutes, Ludhiana, Punjab, 142021
komalrani9811@gmail.com

ABSTRACT

Precision oncology aims to improve cancer treatment by identifying molecular alterations that influence tumour development, progression, and therapeutic response. The integration of multi-omics data, including genomics, transcriptomics, proteomics, and metabolomics, provides a comprehensive understanding of tumour heterogeneity and disease-specific molecular pathways. Computer-Aided Drug Design (CADD) can utilize these molecular insights to support the identification and optimization of targeted therapeutic candidates. Genomic and transcriptomic information can assist in identifying cancer-associated mutations and dysregulated targets, while proteomic data may provide information on protein expression and potential druggable targets. Metabolomic profiling can further reveal altered metabolic pathways associated with tumour progression and treatment response. These datasets can guide molecular docking, virtual screening, quantitative structure–activity relationship (QSAR) modelling, molecular dynamics simulations, and ADMET prediction for the rational selection and optimization of drug candidates. Such an integrated approach may facilitate the development of therapies directed toward specific molecular characteristics of cancer subtypes and patient populations. However, challenges related to tumour heterogeneity, multi-omics data integration, target validation, and translation of computational predictions into clinically effective therapies remain significant. Overall, multi-omics-guided CADD represents a promising strategy for precision oncology by linking molecular profiling with rational drug discovery and supporting the development of more targeted and potentially effective anticancer therapies.

Keywords: Multi-Omics, Computer-Aided Drug Design, Precision Oncology, Molecular Docking, Targeted Therapy.

Formulation & Evaluation of Nasal Spray to in situ Nasal Gel of Loratadine

Mr. Debayan Bag[1*], Mr. Sumit Prasad Bhakat[1], Mr. Sourav Bhowmick[1], Prof. (Dr.) Mithun Bhowmick[1]
[1]Bengal College of Pharmaceutical Sciences and Research, Durgapur, 713212, West Bengal
debayanbag02@gmail.com

ABSTRACT

Loratadine, a second-generation antihistamine used to treat allergic rhinitis and urticaria, suffers from poor oral bioavailability due to extensive first-pass hepatic metabolism. Converting the conventional nasal spray into an in situ gelling system offers a promising alternative, since the nasal route bypasses the liver, and a gel that forms only after administration can extend the residence time of the drug on the nasal mucosa, improving both absorption and patient compliance.The in situ nasal gel was formulated using thermosensitive and pH-triggered polymers such as poloxamer 407, HPMC K-100, xanthan gum, and carbopol 934P, often combined to balance gelling behavior with mucoadhesive strength. Formulations were evaluated for clarity, gelling temperature, gelling time, drug content, pH, and mucoadhesive strength to ensure the gel would form appropriately without causing nasal irritation. Additional characterization typically includes viscosity, in vitro drug release, and short-term stability testing. Optimized batches generally show sustained drug release for up to ten hours, following Higuchi release kinetics, with good physical stability over several months and no significant drug-polymer interaction. Advanced approaches incorporating cyclodextrin complexation have further improved drug solubility and achieved near-complete cumulative permeation within a few hours while maintaining strong mucoadhesion. The in situ nasal gel of loratadine appears to be a viable, patient-friendly alternative to conventional oral and spray dosage forms, offering controlled release, prolonged nasal contact, and potentially enhanced bioavailability by avoiding first-pass metabolism.

Keywords: Loratadine, In situ nasal gel, Mucoadhesion, Bioavailability, Controlled drug release, etc.

Formulation Approaches&Recent Advances of Intra Nasal drug delivery system of Donepezil for Alzheimer Disease

Mr. Soumyajit Roy1*, Ms. Debarati Basu1, Dr. Sunanda Tuladhar1, Prof. (Dr.) Mithun Bhowmick1
1Bengal College of Pharmaceutical Sciences and Research, Durgapur, 713212, West Bengal
roysoumyajit444@gmail.com

ABSTRACT

Alzheimer's disease remains one of the most challenging neurodegenerative disorders to treat, largely because the blood-brain barrier limits howmuchdrug actually reaches thebrain. Donepezil, a first-line acetylcholinesterase inhibitor, is widely prescribed orally, but its current oral formulations show reduced bioavailability because of limited permeability across the blood-brain barrier. The intranasal, or nose-to-brain, route has emerged as an attractive alternative because it delivers drugs directly to the central nervous system while bypassing the blood-brain barrier and avoiding first-pass metabolism. This review compiles and analyzes recent formulation strategies reported in review and research articles published between 2022 and 2026, focusing on lipid-based, solid particle-based, solution-based, gel-based, and film-based donepezil delivery systems designed for nasal administration, along with their preclinical evaluation methods. Result Across studies, nanocarrier-based systems consistently outperformed conventional oral dosing. Formulations such as poloxamer lipogels of donepezil demonstrated up to six-fold increases in brain bioavailability alongside improved behavioral outcomes and fewer systemic side effects. Similarly, intranasal liposomal donepezil combined with other agents produced better short-term memory recovery than oral dosing in transgenic Alzheimer's mouse models, while nanoemulsion and dendrimer-based carriers showed favorableparticle size, entrapment efficiency, and sustained-release profiles. Intranasal nanocarrier systems represent a promising, non-invasive strategy to overcome donepezil's oral bioavailability limitations, though most evidence remains preclinical and calls for further pharmacokinetic and long-term human safety studies.

Keywords: Intranasal delivery; Donepezil; Nose-to-brain drug delivery; Alzheimer's disease; Nanocarriers

A Novel Rp-Hplc Strategy for Simultaneous Bioanalyticalestimation of Fluticasone Furoate and Oxymetazolinehydrochloride in Human Plasma

Ekta Ram*, Tapash Jyoti Bhattarai, Dr. Avani Khristi
Parul Institute of Pharmacy, Parul University, POLimda, Vadodara, Gujarat, India -391 760.
ektaram28@gmail.com

ABSTRACT

Fluticasone furoate (FF) and oxymetazoline hydrochloride (OXY) are combined in a nasal spray for the treatment of allergic rhinitis, providing both anti-inflammatory and decongestant effects. Even though there are various analytical methods available for FF and OXY either separately or together in nasal formulations, no bioanalytical method has so far been published for determining them simultaneously in human plasma. In this study, a selective RP HPLC method for the simultaneous determination of FF and OXY in human plasma is developed and validated in accordance with the ICH M10 guidelines. The method involved carrying out chromatographic separation on a Shimadzu LC-2050 i-series system with a C18 column (250 × 4.6 mm, 5 µm), employing a PDA detector at 222 nm (this wavelength was chosen as the isosbestic one on the basis of spectral overlay studies) and maintaining a flow rate of 1.0 mL/min. The mobile phase was optimized by using acetonitrile and a potassium dihydrogen phosphate buffer (at pH 3.0) in varying ratios, the optimization being carried out under both isocratic and gradient elution conditions over several trials. The initial tests demonstrated that OXY could be adequately resolved from the plasma matrix (with a retention time of about 4.6 minutes), whereas FF had a considerably longer retention time (about 16 minutes), which suggests that further refinement of the mobile phase could help reduce the run time and enhance the resolution of both compounds at the same time. Work is still being done to optimize the chromatographic conditions. Initial trials aimed at developing the method show that it is feasible to determine both FF and OXY simultaneously in human plasma using RP-HPLC. Optimization of the mobile phase and full validation in accordance with ICH M10 (with regard to selectivity, linearity, accuracy, precision, sensitivity, and stability) are currently underway in order to establish a reliable bioanalytical method suitable for use in pharmacokinetic studies.

Keywords: Fluticasone furoate, oxymetazoline hydrochloride, human plasma, RP-HPLC, bioanalytical method development, ICH M10.

Computer-Aided Drug Design an Innovative Approach for Accelerating Modern Pharmaceutical Discovery

Ashatai Bhagvan Patil
Department of Pharmaceutical Chemistry, Bombay Institute of Pharmacy & Research, Maharashtra, India
Ashataipatil210@gmail.com

ABSTRACT

The conventional drug discovery process is time-consuming, expensive, and associated with a high attrition rate during preclinical and clinical development. Designing Drugs with Computers a Fresh Way to Make Modern Medicine Discovery Faster, usual way of finding new drugs takes a long time, costs a lot of money and many candidates fail in early lab and human trials. The computer-based method known as CADD has grown into a key tool for finding and improving promising drug candidates more quickly. The present work discusses the application of structure-based and ligand-based CADD approaches in pharmaceutical drug discovery. Before doing heavy lab work, it lets researchers' study how molecules interact, predict how they might act in the body, and tell if they have what it takes to be a medicine. This work looks at how structure-based and ligand-based CADD methods are used to discover new pharmaceutical drugs. Researchers used molecular docking to predict how ligands bind to targets and how strongly and they applied pharmacophore modelling along with QSAR methods to pinpoint the structural traits that drive biological effects. The analysis indicates that integration of CADD techniques can facilitate rapid virtual screening, identification of potential lead molecules, prediction of binding interactions and prioritization of compounds for experimental validation. They also used computer-based ADMET prediction to get an early check on absorption, distribution, metabolism, excretion and toxicity. The findings show that combining CADD methods can speed up virtual screening, help find promising lead compounds, predict how they bind, and rank candidates for lab testing. CADD represents a powerful and innovative component of modern pharmaceutical research. Newer AI-driven computational tools and molecular dynamics simulations were also examined as ways to sharpen predictions and improve lead compounds

Keywords: Computer-Aided Drug Design, Molecular Docking, QSAR, Pharmacophore Modelling, Drug Discovery

Network Pharmacology-Based Approach to Explore Therapeutic Potential of *Aerva lanata* Against Rheumatoid Arthritis

Swati Chaudhry1, Dr. Praveen Kumar Dixit2
1Department of Pharmacology, KIET School of Pharmacy, KIET Deemed to be University, Ghaziabad, Uttar Pradesh, India;
2Associate Professor, Department of Pharmacology, KIET Deemed to be University, Ghaziabad, Uttar Pradesh, India
praveen.dixit@kiet.edu

ABSTRACT

Rheumatoid arthritis is a chronic autoimmune disorder characterized by persistent inflammation of joints. Although DMARDs, biologics and glucocorticoids are the main treatment approaches for RA, these medications are not effective for every patient or do not provide complete and long-term relief. Therefore, network pharmacology was used to determine the effects of *Aerva lanata* on multiple targets in RA, and suggested molecular docking for future validation. To investigate the targets and molecular pathways of anti-arthritic activity in RA using network pharmacology. Data on Aerva lanata were collected from the PubChem and IMPPAT databases. Then, the target prediction platforms were used to predict the potential targets of each compound. The genes associated with RA were selected from the GeneCards database. Common genes between disease-associated genes and predicted phytoconstituent targets were identified and used to construct a PPI network in STRING, which was analyzed in Cytoscape. A pathway enrichment analysis was carried out using the DAVID tool. The PPI network analysis identified seven hub genes, including TNF, AKT1, BCL2, CTNNB1, SRC, EGFR, and HSP90AA1. Enrichment analysis showed that Aerva lanata may exert its therapeutic effects on inflammation by means of a number of pathways, including the MAPK, PI3K-AKT, HIF-1, and JAK-STAT pathways. The indicated that Aerva lanata may act on multiple molecular targets and pathways involved in the pathogenesis of RA, suggesting that Aerva lanata may serve as a promising phytotherapeutic candidate for rheumatoid arthritis management. However, these findings are based on computational analysis and require further validation using molecular docking and experimental studies to establish the interaction of identified compounds with hub targets before use in the treatment of the disease.

Keywords: Rheumatoid Arthritis; Aerva lanata; Network Pharmacology; Bioinformatics; Therapeutic Targets.

Network Pharmacology-Based Identification of Putative Anti-Rheumatoid-Arthritis Targets of Ajuga bracteosaPhytoconstituents A Target Prediction, Disease-Target Intersection, Pathway Enrichment, and ADMET Study

Madhu Raghav, Dr. Praveen Kumar Dixit*
KIET Deemed to be University, Ghaziabad, Uttar Pradesh, India
praveen.dixit@kiet.edu

ABSTRACT

Ajuga bracteosa Wall. ex Benth. is used traditionally for inflammatory and arthritic conditions, and its ethanolic extract has documented cyclooxygenase-inhibitory activity in rodent arthritis models. However, no published study has applied an integrated network pharmacology framework to this species specifically against rheumatoid arthritis (RA). A phytoconstituent inventory of 32 confirmed compounds was compiled from primary isolation/quantification literature on *A. bracteosa*. Of these, 22 compounds with resolvable PubChem structures were submitted to SwissTargetPrediction (probability ≥ 0.1), yielding 228 unique human targets. RA-associated genes were retrieved from GeneCards (top 5% relevance score, n = 416). The intersection (36 common targets) was mapped onto the STRING protein-protein interaction database and analysed using NetworkX for degree, betweenness, and closeness centrality. Gene Ontology and KEGG pathway enrichment were performed using Enrichr with Benjamini-Hochberg FDR correction, and ADMET/drug-likeness was evaluated using SwissADME.The 36 common targets formed a connected network of 302 interactions. TNF, IL1B, STAT3, PTGS2 (COX-2), MMP9, and TLR4 emerged as the most central hub targets. KEGG enrichment identified 129 significant pathways (adjusted $p < 0.05$), prominently TNF signaling, IL-17 signaling, Toll-like receptor signaling, and osteoclast differentiation. GO Biological Process analysis was dominated by regulation of inflammatory response and cytokine production. At least eight compounds, including Withaferin A, Ajugarin I, and Clerodin, showed favourable oral drug-likeness (zero Lipinski violations, high predicted GI absorption, no BBB permeation). This study provides computational, hypothesis-generating evidence that *A. bracteosa* phytoconstituents converge on core RA-relevant inflammatory signaling (TNF/IL-1/IL-17/TLR/osteoclast axes), complementing prior wet-laboratory COX-inhibition findings. Molecular docking and experimental validation are planned as the next phase of this study.

Keywords: *Ajuga bracteosa*; rheumatoid arthritis; network pharmacology; protein-protein interaction; KEGG pathway enrichment; ADMET

Application of AI-Driven Techniques, Molecular Design, Nanotechnology and Virtual Screening Techniques for Alzheimer's Disease A Literature Review

ABSTRACT

Ankur Sharma*[1], Praveen Kumar Dixit[1]
[1]Department of Pharmacology, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Uttar Pradesh
*ankur.26sphd0010@kiet.edu

ABSTRACT

Alzheimer's disease (AD) is a multifactorial neurodegenerative disorder involving amyloid-β aggregation, tau dysregulation, cholinergic dysfunction, neuroinflammation, and oxidative stress. These mechanisms, together with the blood–brain barrier (BBB), limit conventional drug development. Artificial intelligence (AI), molecular design, virtual screening (VS), molecular modelling, and nanotechnology offer complementary strategies for accelerating therapeutic discovery and brain delivery. This review evaluates their applications in potential AD therapeutics. A targeted review of peer-reviewed PubMed-indexed studies was conducted, focusing on computational and experimental research in AI/ML-assisted molecular discovery, VS and molecular simulation, rational molecular design, and nano-enabled brain-targeted drug delivery.AI/machine learning (ML) can analyze large datasets, predict bioactivity, and prioritize compounds for experimental testing. Screening approximately 360,000 compounds identified 88 acetylcholinesterase (AChE) and 126 butyrylcholinesterase (BChE) inhibitors, including novel active scaffolds. ML combined with molecular docking and dynamics has identified stable BChE inhibitors, while deep learning has linked screening of traditional-medicine libraries with biological validation. AlzyFinder enables ligand-based screening across more than 85 AD-associated targets. Structure-based VS integrating pharmacophore modelling, docking, molecular dynamics and free-energy calculations has identified promising AChE and GSK-3β inhibitors with favorable predicted properties, including BBB penetration. Deep-learning docking has enabled ultra-large-library screening, identifying low-nanomolar Aβ42 fibril binders. Polymeric nanoparticles, lipid nanocarriers, and extracellular vesicles may improve drug stability, sustained release, cellular uptake, and BBB transport. Integrating AI, computational design, VS, molecular simulation, and nanotechnology may accelerate AD therapeutic development. However, toxicity, scalability, BBB heterogeneity, and limited clinical validation remain key barriers. Future research should integrate multimodal datasets, explainable/generative AI, BBB-aware optimization, standardized validation, and experimentally validated nanomedicines to advance clinically meaningful disease-modifying therapies.

Keywords: Alzheimer's disease, Artificial intelligence, Machine-learning, Nanomedicine

Comparative Molecular Similarity Indices Analysis to Determine Antidiabetic Activity of Novel Thioglitazones

Aayush Bhattacharya[1], BR Prashantha Kumar[1*]
[1]Department of Pharmaceutical Chemistry, JSS College of Pharmacy, JSS Academy of Higher Education and Research, Mysore, 570015
brprashanthkumar@jssuni.edu.com

ABSTRACT

Type 2 diabetes mellitus is a widespread global disease marked by reduced insulin secretion and insulin resistance. Peroxisome proliferator-activated receptor gamma (PPAR-γ) agonists, particularly thiazolidinediones (thioglitazones), help to improve glucose metabolism and enhance insulin sensitivity. However, developing new PPAR-γ agonists through rational design still depends on a better understanding of their structure-activity relationships. Using Comparative Molecular Similarity Indices Analysis (CoMSIA), a 3D-QSAR technique, to study thioglitazones helps to determine structural features that control antihyperglycemic activity and establish design guidelines for developing new PPAR-γ agonists. A collection of 50 thioglitazones was split into a training set of 39 compounds and a test set of 11 compounds. Antihyperglycemic activity was normalized and reported as lnMHGA. Molecular structures were optimized using SYBYL 6.7, aligned to a thiazolidinedione scaffold, and evaluated for steric, electrostatic, hydrophobic, hydrogen-bond donor, and hydrogen-bond acceptor properties. Predictive models were then built and assessed using partial least squares regression, cross-validation, and bootstrapping. The optimized CoMSIA model using combined SEHDA fields yielded $q^2 = 0.51$, $r^2 = 0.942$, and test predictive $r^2 = 0.849$ on the test set. The relative contributions of fields were steric 36.8%, electrostatic 22.2%, hydrophobic 21.3%, hydrogen-bond donor 8.0%, and acceptor 11.7%. The contour maps indicated that a 5-benzyl-1,3-thiazolidine-2,4-dione scaffold, an ether oxygen directly attached to the aromatic ring, and a two-carbon linker between the oxygen and terminal rings are critical for activity. In contrast, longer linkers or absence of ether oxygen decrease potency. Hydrophobic groups have enhanced activity when positioned in favorable regions, whereas poorly positioned substituents weakened it. CoMSIA accurately predicted antihyperglycemic activity of thioglitazones and identified key structural features that influence this effect. The validated model offers rational design guidelines for optimizing PPAR-γ agonists and supports the development of improved therapeutic agents for type 2 diabetes.

Keywords: Anti-hyperglycemic, Thioglitazones, PPAR-γ agonists, Type 2 diabetes mellitus, 3D-QSAR

Analytical study of Polmacoxib using UV and HPLC method

Siddhi K. Upadhyay, Prof. Kiran R. Rathod
School of Pharmacy, Dr. Subhash University, Gujarat, India
sidu4932@gmail.com

ABSTRACT

Polmacoxib is a new NSAID drug, which is used for the treatment of pain and inflammation in osteoarthritis. From quality control and quantitative estimation point of view, simple, accurate, precise, sensitive and reproducible analytical methods are very essential for the estimation of polmacoxib in pharmaceutical formulations. The purpose of the present study is to develop and validate the analytical methods of polmacoxib by ultraviolet-visible (UV-Visible) spectrophotometry and high-performance liquid chromatography (HPLC). In the case of spectrophotometric method, the appropriate solvent was chosen and the absorption spectrum of polmacoxib was obtained to determine the wavelength of maximum absorption. The method was tested for linearity, accuracy, precision and sensitivity in the selected range of concentrations. A suitable C18 column, optimized mobile phase, appropriate flow rate and UV detection were used in the chromatographic method. The proposed HPLC method was tested for system suitability, specificity, linearity, accuracy, precision and robustness following applicable ICH analytical validation principles. The successful estimation of polmacoxib by UV spectrophotometry includes the zero-order method with λmax reported at 316 nm, and RP-HPLC method with UV detection at about 238–240 nm. The comparison between the two analytical methods shows the merits of using simple and economical UV spectrophotometry technique as a more selective and reliable HPLC technique for pharmaceutical analysis. The analytical procedures developed may be useful for routine quality-control testing and quantitative estimation of polmacoxib in bulk drug and pharmaceutical dosage forms provided they are confirmed with the experimental data obtained in the present study.

Keywords: Ultraviolet-visible (UV-Visible) spectrophotometry, high-performance liquid chromatography (HPLC), spectrophotometric method, analytical validation principles.

QUALITY DRIFT DETECTING SMALL PROCESS CHANGES BEFORE THEY BECOME MAJOR DEVIATIONS

Dinesh Jepar
M.Pharm, Semester 3, Dr. Subhash University, Junagadh
Mentor Dr. Hiral S. Popaniya
dineshjepar777@gmail.com

ABSTRACT

Quality drift refers to the gradual movement of a process or product characteristic away from its established state of control, even when individual is still within specification. Although these changes may appear minor, repeated shifts can increase process variability and eventually result in OOS or OOT, deviations, batch rejection, complaints, and regulatory concerns. Early recognition is therefore important for maintaining consistent product quality. The presentation describes a proactive approach for detecting and managing quality drift throughout the product lifecycle. Critical Process Parameters, Critical Quality Attributes, in-process controls, and environmental parameters are first identified and a historical baseline is established. Data from batches, equipment, laboratory testing, environmental monitoring, deviations, and complaints are then collected and trended. Control charts, process capability measures such as Cp and Cpk, OOT trending, APQR, and Continued Process Verification are used to identify changes in process behaviour. Observed trends are assessed according to risk, followed by investigation and early intervention when required. The framework shows that useful warning signs can be identified before a specification failure occurs. These include increasing variability, gradual mean shifts, repeated minor deviations, rising rejection rates, environmental changes, and unusual that remain within specification. In the sterile filling case study, an upward fill-weight trend was detected before a major deviation, allowing review of equipment performance, calibration, process parameters, and other possible causes. Corrective action followed by enhanced monitoring helped return the process toward its historical state. Quality drift should not be managed only after a failure occurs. Regular trending and review of multiple data sources provide an opportunity to recognize small changes early and respond in a proportionate, risk-based manner. A proactive approach can strengthen the state of control, reduce variability and batch losses, and support continuous improvement in pharmaceutical manufacturing.

Keywords: Quality drift, OOT, process trending, process capability, CPV, APQR, risk assessment, CAPA, pharmaceutical quality.

Analytical Method and Validation of Zolpidem Tartrate by UV Spectrophotometry and RP-HPLC

Himanshu R. Parmar, Prof. Arti Bhetariya
School of Pharmacy, Dr. Subhash University, Gujarat, India
parmarhimanshu713@gmail.com

ABSTRACT

Zolpidem tartrate is a short-acting imidazopyridine hypnotic that is widely used for short-term treatment of insomnia. It is critical to use reliable analytical methods to ensure the quality, potency and uniformity of Zolpidem pharmaceutical compositions. The present study is aimed at the analytical evaluation of Zolpidem tartrate by two methods namely ultraviolet (UV) spectrophotometry and reversed-phase high performance liquid chromatography (RP-HPLC). A review of published studies involving the use of Zolpidem was carried out in order to sum up the analytical conditions and the validation performances of both techniques. Methods based on UV spectrophotometric data have been reported as simple, rapid and economic and are found as suitable quantitative estimation of Zolpidem in bulk drug and tablet formulations. The spectrophotometric procedures all showed linear responses over the concentration ranges of 5–30 µg/mL, 10–50 µg/mL, and 5–40 µg/mL, depending on the method used. The determination of Zolpidem by RP-HPLC methods has been carried out with C18 stationary phases and UV or photodiode-array detection, which is performed in a selective and quantitative way. The RP-HPLC method reported by Akula et al. showed good linearity (10–70 µg/mL), accuracy, precision, robustness, sensitivity and assay. According to the literature reviewed, parameters for validation were linearity, accuracy, precision, specificity, robustness, system suitability, limit of detection, limit of quantification and assay. Based on comparative evaluation, it can be concluded that UV spectrophotometry is simple and economical to operate, while RP-HPLC has a better chromatographic separation and analytical specificity. Overall, both techniques are suitable for a routine pharmaceutical analysis and quality control of Zolpidem tartrate according to the published evidence. The present book offers a narrow analytical outlook of UV spectrophotometric and RP-HPLC methods to be utilized for the accurate determination of Zolpidem present in pharmaceutical preparations.

Keywords: Zolpidem tartrate; ultra-violet (UV-visible) spectrophotometry; High-performance liquid chromatography (RP-HPLC); Method validation; Pharmaceutical analysis.

A Comprehensive Review of Analytical Methods for Imeglimin Hydrochloride and Sitagliptin Phosphate

Shivani P. Herma, Prof. Kiran R. Rathod
School of Pharmacy, Dr. Subhash University, Gujarat, India
Shivaniherma2003@gmail.com

ABSTRACT

Imeglimin hydrochloride and sitagliptin phosphate are oral antidiabetic drugs used for the treatment of type 2 diabetes mellitus. Accurate, precise, sensitive, and reliable analytical methods are essential for the estimation and quality control of these drugs in pharmaceutical formulations. The present review summarizes the reported analytical methods for imeglimin hydrochloride and sitagliptin phosphate, with emphasis on UV-Visible spectrophotometry and reverse-phase high-performance liquid chromatography (RP-HPLC). The review includes important analytical parameters such as wavelength of maximum absorption, solvent, chromatographic column, mobile phase, flow rate, retention time, linearity, accuracy, precision, and other validation parameters. Reported UV-Visible methods utilize suitable absorption wavelengths, while RP-HPLC methods commonly employ C18 columns with UV detection at drug-specific wavelengths (245–275 nm, 266 isosbestic point). The reported methods are compared with respect to their simplicity, accuracy, sensitivity, selectivity, and suitability for routine pharmaceutical quality-control analysis. This review provides useful information on the available analytical methods for the estimation of imeglimin hydrochloride and sitagliptin phosphate in bulk drugs and pharmaceutical formulations.

Keywords: Imeglimin hydrochloride, sitagliptin phosphate, anti-diabetic drugs, ultraviolet-visible (UV-Visible) spectrophotometry, high-performance liquid chromatography (HPLC), spectrophotometric method, analytical validation principles

Quality 4.0 in the Pharmaceutical Industry Transformation of Pharmaceutical Quality Management Systems through Digitalization, AI and Data Analytics

[1]Mr. Harsh H. Madiya, [2]Dr. Hiral S. Popaniya
[1,2]School of Pharmacy, Dr. Subhash University, Junagadh, Gujarat, India
harshmadiya@gmail.com

ABSTRACT

Reactive quality management is giving way to linked, data-driven, proactive systems in the pharmaceutical sector. By fusing digital technology with Pharmaceutical Quality Management Systems (PQMS), Good Manufacturing Practices (GMP), Quality by Design (QbD), and continuous improvement, Quality 4.0 embodies this change. Pharmaceutical quality operations are being impacted by artificial intelligence (AI), machine learning, cloud computing, digital twins, big data analytics, Internet of Things (IoT), and Process Analytical Technology (PAT). In order to learn more about technology utilization, quality enhancements, implementation challenges, and regulatory concerns, this evaluation focused on recent research on quality 40 and its application to pharmaceutical quality management from 2023 to 2026. We looked at peer-reviewed research reviews and regulatory sources. AI-based quality assurance predictive analytics, data integrity real-time monitoring, digital quality management systems, and regulatory compliance received special attention. According to the literature, Quality 4.0 can enhance pharmaceutical quality by enabling data-driven decisions, real-time data gathering, predictive quality monitoring, early problem detection, predictive maintenance, and improved traceability. Finding anomalies, streamlining procedures, forecasting quality, automating paperwork, and auditing quality management systems are all aided by AI and machine learning. Controlling crucial quality aspects and process parameters ahead of time is another benefit of using IoT, analytics, and PAT. Companies still have to deal with obstacles including outdated systems, disparate data sources, incompatibility, cybersecurity threats, poor data quality, a lack of digital expertise, expensive expenses, and ambiguous rules. Additionally, risk-based validation, model management, documentation, traceability, explainability, and robust human oversight are required for AI. Quality 4.0 is a change in pharmaceutical quality culture, procedures, and decision-making rather than only a technological advancement. Aligning technology, personnel, procedures, data governance, and legal requirements is necessary for its implementation. Pharmaceutical companies can transition from reactive quality management to predictive, integrated, and continuously improving quality management while ensuring patient safety and regulatory compliance by using a risk-based and lifecycle approach to Quality 4.0 implementation.

Keywords: Quality 4.0; Pharmaceutical Quality Management System; Artificial Intelligence; Data Analytics; Digitalisation; Regulatory Compliance; Data Integrity; Predictive Quality; GMP.

From Reactive to Predictive Quality Assurance Machine Learning-Based Prediction of Recurring Deviations and CAPA Effectiveness in Pharmaceutical Manufacturing

Jadav Krupali
Guide Dilnaz Kadri | Co-Guide Kiran Rathod
School of Pharmacy, Dr. Subhash University, Gujarat, India
Krupalijb016@gmail.com

ABSTRACT

Pharmaceutical Quality Assurance (PQA) is gradually moving from a reactive approach toward earlier identification of recurring quality risks. Deviations are followed by investigation, root-cause analysis, corrective and preventive action (CAPA), and effectiveness checks. Although these activities are essential for Good Manufacturing Practice (GMP), repeated deviations may indicate inadequate root-cause control or ineffective CAPA. This review examines how machine learning (ML), Quality Management System (QMS) data, manufacturing signals, and natural language processing (NLP) may support predictive QA. Recent research indicates that historical deviation records contain valuable information for identifying recurring problems and similar incidents. ML-based anomaly detection can assist in recognizing abnormal manufacturing behaviour, while NLP and text-embedding techniques can support analysis of investigation narratives. However, an integrated framework linking recurring deviations with CAPA effectiveness remains insufficiently validated. A focused literature review was conducted covering pharmaceutical deviations, CAPA effectiveness, predictive quality, ML, anomaly detection, NLP, QMS analytics, and GMP implementation of AI/ML. Published research was grouped into recurrent-deviation management, CAPA effectiveness, ML-based process monitoring, and NLP-based deviation analysis. These findings were synthesized into a conceptual predictive-QA framework. The reviewed evidence suggests that deviation frequency, severity, batch and equipment history, OOS/OOT events, previous CAPAs, root-cause categories, effectiveness-check outcomes, and investigation text could be combined to identify patterns associated with recurrence. Such a system could prioritize high-risk cases for further QA review. However, implementation requires reliable data, validation, explainability, cybersecurity, data integrity, and appropriate GMP controls. ML has potential to transform historical quality records into forward-looking quality intelligence. Integrating QMS data, CAPA history, manufacturing signals, and investigation text may support earlier identification of recurring risks and improve CAPA effectiveness monitoring. Future research should validate the proposed approach using real electronic QMS datasets while maintaining qualified human oversight and regulatory compliance.

Keywords: Machine Learning; Artificial Intelligence; Pharmaceutical Quality Assurance; Quality Management System; Recurring Deviations; CAPA; CAPA Effectiveness; Predictive Quality Assurance; Anomaly Detection; Natural Language Processing; GMP.

Repurposing of Statins-Development, Characterization and Evaluation of Statin loaded nanoparticles

Mohd Shahnawaz[1], Dr. Prasoon kumar saxena[2]
School of Pharmaceutical Sciences, SDGI Global University Ghaziabad
shanubpharm007@gmail.com

ABSTRACT

Statins are widely used lipid-lowering agents and play an important role in the prevention and management of cardiovascular diseases. However, their therapeutic effectiveness may be limited by poor aqueous solubility, low bioavailability, extensive first-pass metabolism, and dose-related adverse effects. Nanotechnology-based drug delivery systems offer a promising approach for improving the physicochemical and pharmacokinetic properties of poorly soluble drugs. The present research is aimed at the development and characterization of statin-loaded nanoparticles, particularly using atorvastatin and/or fluvastatin, to enhance drug solubility, dissolution, bioavailability, and therapeutic performance. The nanoparticles will be prepared using an appropriate nanoparticle fabrication technique and suitable biocompatible polymers or stabilizers. The developed formulations will be evaluated for particle size, polydispersity index, zeta potential, morphology, drug entrapment efficiency, drug loading, and physicochemical compatibility. In-vitro drug release and release kinetics will be investigated to determine the drug-release behavior of the optimized formulations. Stability studies will also be performed under suitable storage conditions. The optimized statin-loaded nanoparticles are expected to provide improved drug dissolution and controlled/sustained drug release compared with the conventional drug formulation. The proposed study may provide a promising nanocarrier-based approach for improving the delivery of statins and potentially enhancing their therapeutic efficacy while reducing dose-related limitations. The developed formulation may serve as a potential platform for further pharmacokinetic, pharmacodynamic, and in-vivo evaluation.

Keywords: Statins, Atorvastatin, Fluvastatin, Nanoparticles, Nanocarriers, Drug Delivery, Bioavailability, Controlled Release.

Intelligent Quality Management Systems The Role of Artificial Intelligencein Next-Generation Pharmaceutical Quality Assurance

Dev J. Solanki, Prof. Khushbu H. Parmar, Dr. Hiral Popaniya
School of Pharmacy, Dr. Subhash University, Gujarat, India
devsolanki374@gmail.com

ABSTRACT

Pharmaceutical Quality Assurance (PQA) is experiencing a paradigm shift, marked by a shift towards cutting-edge technologies such as Artificial Intelligence (AI), machine learning, and automation, as well as advanced data analysis tools. The majority of QA practices are based on manual review, periodic testing, review of documentation and a reactive audit of deviations. This review explores how artificial intelligence (AI) and automation can contribute to the improvement of the pharmaceutical Quality Management Systems (QMS) and solve quality, compliance, efficiency and patient safety challenges. Predictive analytics can be used to detect any process or equipment anomalies early in the process and take preventive and corrective measures before the large problems occur to maintain quality. Computer vision and automatic visual inspection with AI can boost defect detection, contamination, packaging defects and labelling errors and reduce the variability of manual inspection. Further applications such as Natural Language Processing, Pattern recognition, Anomaly detection and AI-assisted Root cause can also support the quality investigation and evidence-based decision making. Other traceability tools, data integrity, process control and operation efficiencies achieved through automation include Robotic Process Automation, Electronic Batch Records, Supervisory Control and Data Acquisition systems, Manufacturing Execution Systems, robotics and IoT based monitoring. When it comes to patient-related or quality-critical processes, ethics and a need for human-in-the-loop decision making are particularly significant when it comes to AI. In, where AI and automation are well understood and validated and implemented according to GxP requirements and Pharma 4.0 principles, they can contribute to shifting the focus of pharmaceutical quality management from reactive to proactive, predictive, consistent, and data-driven, whilst upholding product quality, regulatory compliance, and patient safety.

Keywords: Artificial Intelligence, Predictive Analytics, Automation, Computer Vision, Pharma 4.0 principles, Electronic Batch Records, Robotic Process Automation

Pharmacological and Therapeutic Potential of Harpagophytum procumbens (Devil's Claw) in Inflammatory Disorders an Integrated In-Silico, In-vitro, In-vivo and Mechanistic Investigation

Rajat Panwar[1], Dr. Praveen Kr. Dixit[2]

1 PHD Scholar, Department of Pharmacology, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India; rajatpanwar2320@gmail.com

2 Associate Professor, Department of Pharmacology, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India; praveen.dixit@kiet.edu

ABSTRACT

Devil's claw, or *Harpagophytum procumbens subsp. procumbens,* is a prominent medicinal plant of the Pedaliaceae family (sesame seed family). Most of it is dispersed throughout southern Africa. Its remarkable reputation stems from its historic use as an indigenous herbal remedy for syphilis, bitter tonic, inflammatory febrifuge, menstruation issues, and even appetite loss. Many bioactive substances have been identified, including terpenoids, glycosides, iridoid glycosides, and acetylated phenolic compounds. Numerous phytochemical investigations have indicated the bioactive chemicals harpagoside and harpagide, iridoid glycosides, as possible analgesics, and pain relievers. Numerous ailments, including Alzheimer's disease, obesity, rheumatoid arthritis, type 2 diabetes, cancer, cardiovascular, and pulmonary disorders have been linked in-depth research to chronic inflammation. Furthermore, chronic inflammatory disorders account for 60% of chronic disorder-related deaths globally. Significant attention has been paid to inflammation and diseases associated to pain as the primary drivers of global health issues. It is also clear that in vivo clinical research is still required to confirm the anti-inflammatory and analgesic effects of *H. procumbens* compounds. The pharmacological properties and therapeutic potential of *Harpagophytum procumbens* will be thoroughly reviewed in this session, with a focus on how it may be used to treat inflammatory disorders like arthritis. The findings underscore the relevance of natural products as viable choices in current pharmacotherapy.

Keywords: *Harpagophytum procumbens*, Devil's Claw, inflammation, arthritis.

Enhancing Transdermal Delivery of Terbinafine Development and Evaluation of a Transfersomal Emulgel

N. Harini*, H. Gayathri
Department of Pharmaceutics, SRM College of Pharmacy, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India
harini.n.pai05@gmail.com

ABSTRACT

The present study aimed to enhance the transdermal delivery of terbinafine hydrochloride by developing a transfersomalemulgel for effective management of dermatophytosis. Terbinafine, though a potent antifungal agent, exhibits poor aqueous solubility and limited permeability across the stratum corneum, restricting its therapeutic efficiency in topical formulations. Transfersomes, ultra-deformable phospholipid vesicles containing edge activators, were employed to overcome these limitations. Terbinafine-loaded transfersomes were prepared using thin film hydration method and were optimized using a Box–Behnken design by evaluating phosphatidylcholine, sodium deoxycholate, and solvent ratio effects on particle size, entrapment efficiency, and polydispersity index. The optimized formulation exhibited vesicle size <200 nm, PDI <0.3, and entrapment efficiency >80%. The suspension was incorporated into a Carbopol-based emulgel showing suitable pH, viscosity, spreadability, and drug content. In vitro release demonstrated sustained release for 12h following Higuchi kinetics. Ex vivo permeation across rat skin showed significantly enhanced flux (35.7 ± 2.1 µg/cm²/h) and permeability coefficient (1.21 × 10^{-3} cm/h) compared to conventional cream. Antifungal studies against Trichophyton rubrum showed a larger inhibition zone (27.9 ± 1.1 mm). Skin irritation and stability studies confirmed safety and formulation robustness. The trasfersomalemulgel demonstrated enhanced permeation, sustained release, superior antifungal efficacy, and stability, indicating its potential as an advanced topical drug delivery system.

Keywords: Transfersomes; Nanotechnology; Advanced drug delivery; Computational formulation; Emulgel; Terbinafine; Transdermal delivery; Antifungal therapy; Drug permeation

From reactive to predictive quality Critical Review of ICH Q9 (R1)- Risk based CAPA management and emerging data driven approaches

[1]Pranjal Ramrakhiyani ,[2]Prof. Kiran Rathod
[1,2]School of Pharmacy, Dr. Subhash University, Junagadh, Gujarat, India
ramrakhiyanipranjal@gmal.com

ABSTRACT

Historically, pharmaceutical quality management has taken a reactive strategy, investigating deviations, failures, and complaints after they happen and taking corrective and preventative action (CAPA). A more proactive and predictive quality system is becoming more and more necessary as risk-based decision-making and continuous improvement are prioritized. This research investigates new data-driven strategies for bolstering pharmaceutical quality systems and critically evaluates the application of ICH Q9(R1) principles to risk-based CAPA management. We examined and contrasted pertinent published literature and regulatory recommendations on quality risk management, CAPA, root-cause analysis, predictive quality, artificial intelligence, machine learning, process monitoring, and digital technologies. According to the literature, combining quality risk management with CAPA can boost preventative measures, facilitate more organized investigations, and enhance the prioritization of quality events. However, traditional CAPA procedures may not be able to sufficiently identify emerging or recurrent hazards prior to quality incidents since they mostly rely on previous data. Recent developments in process analytical technology, machine learning, artificial intelligence, data analytics, and real-time monitoring offer chances to spot trends, identify process variability, anticipate possible quality problems, and facilitate early intervention. Despite these advantages, issues with data availability, data integrity, model dependability, validation, cybersecurity, and technological know-how must be resolved before broad use. Overall, the shift from reactive quality management to predictive and continuously improving pharmaceutical quality systems may be supported by combining ICH Q9(R1)-based risk management, efficient CAPA systems, and dependable data-driven technologies.

Keywords: ICH Q9(R1), Quality Risk Management, CAPA, Root Cause Analysis, Predictive Quality, Data Analytics, Machine Learning, Pharmaceutical Quality System.

Repositioning of Epigallocatechin Gallate-Loaded Nanolipid Carrier Targeting Vascular Endothelial Growth Factor VEGF for the Management of Retinal Neovascularization by Non-Invasive Route

[1]Kousalya Selvaraj

Department of Pharmaceutics, Amity Institute of Pharmacy, Amity University, Bengaluru, Karnataka, India

kousalyapharma@gmail.com

ABSTRACT

Diabetic retinopathy (DR) is one of the most common complications, and approximately 80% of patients with diabetes for over ten years suffer from some degree of DR. Due to high cost, invasive procedure, highlights the importance of developing an alternative approach. Hence, there is a need to develop alternative drug delivery. Currently many pharmaceutical companies focusing on drug repositioning rather than new drug discovery because of its cost and time consumption. Considering that, I have selected the Epigallocatechin-Gallate (EGCG) due to its potent anti-angiogenic activity and antioxidant and anti-inflammatory activity for the management of DR. EGCG-loaded NLCs were prepared using the microemulsion technique. The influence of lipid concentration, surfactant concentration, and homogenization time on particle size, polydispersity index (PDI), and entrapment efficiency was systematically investigated to obtain an optimized formulation. The optimized NLCs were further characterized for particle size, PDI, surface morphology, entrapment efficiency, *in vitro* drug release, and ocular irritation using the hen's egg test–chorioallantoic membrane (HET-CAM) assay. The formulation variables had a pronounced effect on the physicochemical characteristics of the NLCs. The optimized formulation exhibited favourable particle size, narrow size distribution, and high drug entrapment efficiency. The optimized NLCs showed a rapid drug release profile over 2 hours and were found to be non-irritant in the HET-CAM assay, indicating good ocular compatibility. The optimized EGCG-loaded NLC exhibited desirable physicochemical properties, efficient drug encapsulation, satisfactory release behaviour, and good ocular safety. Overall, this formulation represents a promising platform for improving the ocular delivery of EGCG and may offer a potential therapeutic strategy for the management of diabetic retinopathy.

Keywords: Epigallocatechin gallate; nanostructured lipid carriers; diabetic retinopathy; ocular drug delivery

Evaluation of Anti-hyperlipidemic Activity of *Dillenia indica* L stem and *Limoniaacidissima* Linn Root Extract in edible oil induced hyperlipidemia model rats

Salema Khatun[1], Saikat Sen[2]
Department of Pharmacology, School of Pharmaceutical Sciences, Girijananda Chowdhury University, Azara, Guwahati, Assam, India, PIN – 781017.
salemakhatun316@gmail.com

ABSTRACT

In recent years traditional medicinal plants gain importance for the management of metabolic diseases as conventional drugs are not economical, associated with severe side effects and less availability. This study was to investigate the antihyperlipidemic activity of *Dillenia indica* L stem and *Limoniaacidissima* Linn Root extract in edible oil induced hyperlipidemic rats. Hyperlipidemia was induced in rats by feeding Coconut oil and Banaspati ghee (11 ratio) at dose of10 ml/kg body weight for 38 days. Treatment with extract (200 and 400mg/kg, p.o) and standard drug atorvastatin (10mg/kg, p.o.) were given for 21 days after induction of hyperlipidemia. Blood sample were collected from all animals and estimated biochemical parameters using standard diagnostic kits after experimental period. Hyperlipidemia significantly increased serum total cholesterol, triglycerides, LDL-c, VLDL-C and decreased HDL-c concentration. The Extract (200mg/kg, p.o. and 400mg/kg, p.o.) significantly increased HDL-c and decreased total cholesterol, triglycerides, LDL-c and VLDL-C. The extract treatment also reduces the liver enzyme level AST, ALP and ALT indicates hepatoprotective activity, and also reduces creatinine and Blood urea nitrogen indicates protective effects on kidney. It can be concluded that the extract demonstrated significant antihyperlipidemic activity in rats and may serve as a potential herbal therapeutic agent for the management of hyperlipidemia.

Keywords: *Dillenia indica* L, *Limoniaacidissima*Linn, hyperlipidemia, lipid profile, liver function test, kidney function test

Nanostructured Lipid Carriers for Topical Management of Psoriasis Current Advances, Challenges, and Future Perspectives

Zeel Amitbhai Patel[1], Dr. Rajesh Dodiya[1]
[1]*Department of Pharmaceutics, School of Pharmacy, Parul University, Vadodara, Gujarat, India*
zeelpatel7684@gmail.com

ABSTRACT

Psoriasis is a type of autoimmune inflammatory dermatosis, which is connected with the excessive proliferation and differentiation defects and malfunction of skin barrier, making topical treatment ineffective. As for the conventional therapy methods like corticosteroids, vitamin D derivatives, retinoids, calcineurin inhibitors, they suffer from poor penetration, poor drug retention, frequent use, and long-term side effects. The nanostructured lipid carriers (NLCs) can be regarded as the innovative way of enhancing the efficacy of topical drugs by providing increased capacity of drug entrapment, increased release, penetration, and retention. The comprehensive review of scientific literature sources published between 2020 and 2026 was conducted. The sources were analyzed for their content related to the structure, methods of synthesis and processing, physical and chemical properties, mechanism of skin penetration, therapeutic usage, and future perspectives of NLCs. In the analyzed literature, NLCs showed higher drug entrapment capacity, increased release, skin penetration and retention and better efficacy in comparison with conventional topicals. NLCs-based hydrogels have demonstrated the improved physicochemical stability and promising therapeutic effects in preclinical models of psoriasis. Nanostructured lipid carriers represent an innovative method to improve the therapeutic efficiency. Further work in this field should be done in such spheres as manufacturing on large scale, clinical trials, and regulatory issues.

Keywords: Psoriasis; Nanostructured Lipid Carriers; Topical Drug Delivery; Hydrogel; Nanomedicine.

Impact of stress conditions on the stability of fixed-dose combination of Cefpodoxime proxetil and Ofloxacin tablets A stability-indicating rp-hplc study

Pushpendu Gaurav*, Sonal Dubey, Prashant Tiwari
College of Pharmaceutical Science, Dayananda Sagar University, Bengaluru, 562112, Karnataka, India
pushpendu.gaurav-rs-pha@dsu.edu.in

ABSTRACT

Fixed-dose combination (FDC) tablets of Cefpodoxime proxetil and Ofloxacin are extensively used in the treatment of bacterial infections. Forced degradation studies are essential to establish product stability and develop a stability-indicating analytical method as per ICH Q1A (R2) and ICH Q2 (R2) guidelines. Forced degradation studies were performed under acidic, alkaline, oxidative (hydrogen peroxide), thermal, photolytic, and humidity stress conditions. Samples were analysed on a validated RP HPLC method using an ODS C18 column (250 × 4.6 mm, 5 µm). The mobile phase was phosphate buffer (pH 3.0), acetonitrile and methanol (452035, v/v/v) at the flow rate of 0.8 mL/min. The detection was performed at 235 nm. This showed that peroxide exposure had the greatest effect on the stability of the formulation compared to other stress conditions investigated. Cefpodoxime proxetil was found to be more prone to oxidative degradation than Ofloxacin but comparatively less degradation was observed under acid, alkali, thermal, photolytic and humidity stress. Oxidative degradation was found to be the most important degradation pathway for Cefpodoxime–Ofloxacin tablets, which emphasizes the significance of controlling peroxide impurities in excipients, manufacturing processes, packaging materials, and storage conditions.

Keywords: Forced degradation, Cefpodoxime proxetil, Ofloxacin, Fixed dose combination, Oxidative degradation, Hydrogen peroxide.

From *in silico* and machine learning model to validation discovery of novel amide-functionalized imidazopyridines as PIM-1 kinase inhibitors using an integrated ligand and structure-based hopping approach

Vinayak Walhekar[1,2*], Ravindra Kulkarni[3*]

[1]*Dyaan Prasad Global University, School of Pharmacy and Research, Pimpri, Pune, Maharashtra, India*

[2]*Dr. D. Y. Patil Unitech Society's, Dr. D. Y. Patil Institute of Pharmaceutical Sciences and Research, Pimpri, Pune, Maharashtra, India*

[3]*Department of Pharmaceutical Chemistry, BVDU'S Poona College of Pharmacy, Erandawane Pune-411038, Maharashtra, India*

vinayakwalhekar64@gmail.com

ABSTRACT

Proviral integration site for Moloney murine leukemia virus 1 (PIM1) is a constitutively active serine/threonine kinase implicated in oncogenic signaling pathways governing cell proliferation, survival, and apoptosis. Dysregulated PIM1 expression is frequently associated with tumor progression and therapeutic resistance, rendering it an attractive target for the development of targeted anticancer agents. However, no selective PIM1 inhibitor has yet received clinical approval. This study aimed to identify novel PIM1 kinase inhibitors incorporating the imidazo[1,2-*a*] pyridin-2-yl) phenyl) benzamide pharmacophore through a rational pharmacophore based virtual screening strategy, followed by synthesis and comprehensive biological evaluation. A ligand-based pharmacophore model was employed for virtual screening to identify structurally diverse hit molecules. Selected derivatives were synthesized, structurally characterized, and evaluated for antiproliferative activity against HT-29, PC3, and A549 cancer cell lines. The lead compounds were further investigated for PIM1 kinase inhibition, apoptosis induction, and in silico pharmacokinetic profiling, including ADME, drug likeness, and hepatotoxicity prediction. Structure activity relationship studies identified compound 6h as the most potent analogue. It exhibited pronounced antiproliferative activity against HT-29, PC3, and A549 cells and significantly induced apoptosis in HT-29 cells. Compound 6h demonstrated 34.5 ± 3.4% inhibition of PIM1 kinase activity. Furthermore, computational ADME analysis predicted favourable oral drug likeness, 91.15% human intestinal absorption, and an acceptable safety profile with no predicted hepatotoxicity. The integrated computational, synthetic, and biological investigations establish compound 6h as a promising lead scaffold for further lead optimization toward the development of selective PIM1 kinase targeted anticancer therapeutics.

Keywords: PIM-1 kinase, HT-29, Apoptosis, Pharmacophore modelling, Molecular dynamics simulation, Molecular docking

Polypharmacological Potential of Calocybe indica in Depression a Multi-Target Therapeutic Perspective

Dilsar Gohil[1], Rajesh Maheshwari[1]
1Department of Pharmacy, Sumandeep Vidyapeeth deemed to be University, Vadodara, Gujarat, India,
gohildilsr9624@gmail.com

ABSTRACT

Depression is a complex and multifactorial neuropsychiatric disorder involving dysregulation of monoaminergic neurotransmission, hypothalamic–pituitary–adrenal (HPA) axis dysfunction, neuroinflammation, oxidative stress, mitochondrial impairment, and reduced neuroplasticity. Despite the widespread use of conventional antidepressants, their delayed onset of action, incomplete therapeutic response, and associated adverse effects necessitate the exploration of novel therapeutic strategies. Polypharmacology, involving the simultaneous modulation of multiple biological targets by a single therapeutic agent, has emerged as a promising approach for managing complex disorders such as depression. Natural products, particularly medicinal mushrooms, have gained increasing attention because of their diverse bioactive constituents and multi-target pharmacological activities. This review focuses on the existing scientific evidence regarding the polypharmacological mechanisms involved in depression and evaluates the therapeutic potential of Calocybe indica. Particular emphasis is placed on its major bioactive constituents, including phenolic compounds, flavonoids, polysaccharides, ergothioneine, vitamins, and essential minerals. Their potential effects on key pathological mechanisms associated with depression, including serotonergic neurotransmission, HPA-axis signaling, neuroinflammation, oxidative stress, mitochondrial dysfunction, and neurotrophic pathways, were critically examined. The available evidence indicates that Calocybe indica possesses diverse biological activities, including antioxidant, anti-inflammatory, immunomodulatory, and neuroprotective effects. Its bioactive constituents may collectively influence multiple interconnected pathways implicated in depression, thereby supporting its potential as a multi-target therapeutic intervention. The combined modulation of oxidative stress, inflammatory signaling, HPA-axis dysfunction, serotonergic pathways, and neuroplasticity may provide a broader therapeutic effect than single-target approaches. Calocybe indica represents a promising natural candidate for the development of multi-target therapeutic strategies for depression. Its diverse phytochemical profile and potential ability to modulate multiple pathological pathways support further investigation of its antidepressant and neuroprotective properties. However, mechanistic studies, standardized preparations, preclinical validation, and well-designed translational and clinical investigations are required to establish its therapeutic efficacy, safety, and potential role in the management of depression.

Keywords: Calocybe indica; Depression; Polypharmacology; Multi-target therapy; Medicinal mushroom

In Silico CAD Architecture of Bi-Layered Polymeric Scaffolds for Spatial Separation of Incompatible Drug-Excipient Toxicities

*Dr. HariprasadhSelvam
Department of Oral Pathology, Sree Balaji Dental College and Hospital, Tamil Nadu, India
meenuhari4483@gmail.com

ABSTRACT

Fixed-dose combinations (FDCs) are critical tools in modern pharmacotherapy for optimizing patient compliance and therapeutic synergy. However, formulating multiple active pharmaceutical ingredients (APIs) into a single solid dosage unit frequently fails due to chemical incompatibilities. When incompatible APIs or structural excipients physically interact on the shelf, they induce micro-environmental degradation, resulting in toxic impurities. Traditional pharmaceutical manufacturing struggles to prevent these interactions without complex, multi-step coating processes. This study explores an innovative alternative utilizing computer-aided design (CAD) tools to engineer multi-layered architectural scaffolds that physically isolate incompatible components. Aninsilicogeometric model was designed using mechanical computer-aided engineering software to construct a bi-layered core-shell tabletarchitecture. The primary and secondary incompatible drug matrices were computationally mapped into distinct spatial compartments. The computational CAD models successfully optimized a sub-millimeter polymeric shield that maintained absolute spatial separation between the incompatible chemical compartments under storage simulations. The structural simulations confirmed that the CAD-engineered dividing barrier prevented chemical cross-contamination and stopped the formation of toxic degradation products. Furthermore, dissolution fluid dynamics confirmed that the physical architecture allowed independent, sequential release profiles for each API without compromising overall biometric bioavailability. Integrating advanced mechanical CAD tools into solid dosage formulation provides a highly efficient, predictive for mitigating drug-excipient incompatibility toxicities. By treating tablet manufacturing as an architectural engineering problem, pharmaceutical scientists can bypass traditional formulation bottlenecks. This computer-aided design approach accelerates regulatory clearance pathways and introduces a robust paradigm for automated, safe, and personalized multi-drug delivery systems in modern Pharma 4.0 applications.

Keywords: Computer-Aided Drug Design, In Silico Toxicology, Fixed-Dose Combinations, Polymeric Scaffolds, Additive Manufacturing.

Molecular Docking Studies of Nitrogen-Containing Ligands Targeting Plasmodium Species Multi-Target and Multi-Species Perspectives

Priyanka Gupta[1]*, Bhawana Sati[2]
School of pharmacy, Tulas University, Dehradun
Department of Pharmaceutical Chemistry, Banasthali Vidyapeeth, Tonk, Rajasthan
chinuatti@gmail.com

ABSTRACT

Malaria remains a major global health challenge, with *Plasmodium falciparum* and *P. vivax* responsible for most human infections and *P. berghei* serving as an important experimental model. The emergence and spread of antimalarial drug resistance necessitate the discovery of novel compounds with improved efficacy and diverse mechanisms of action. Molecular docking has become an important computational approach in antimalarial drug discovery because it enables prediction of ligand-binding modes, binding affinities, and critical protein–ligand interactions. Nitrogen-containing heterocyclic compounds are particularly attractive owing to their structural diversity and broad pharmacological potential. This review systematically examines molecular docking studies of nitrogen-containing ligands against key *Plasmodium* targets, including dihydrofolate reductase (DHFR), falcipains (FP-2 and FP-3), plasmepsins (PM II, PM III/HAP, and PM X), *P. falciparum* ATPase 4 (PfATP4), and lactate dehydrogenase (LDH). Particular emphasis is placed on Protein Data Bank (PDB) structures, identification numbers, binding-site characteristics, interacting amino acid residues, and predicted binding affinities to facilitate reproducibility and comparative analysis. Cross-species docking involving *P. falciparum*, *P. vivax*, and *P. berghei* provides valuable insights into target conservation and the potential development of broad-spectrum antimalarial agents. Inclusion of *P. berghei* LDH (PbLDH; PDB ID 1OC4) further strengthens the comparative assessment of ligand activity across parasite species. Collectively, the reviewed findings demonstrate the utility of molecular docking for identifying promising scaffolds, understanding structure–activity relationships, and supporting multitarget antimalarial drug design. Integration of docking with molecular dynamics, QSAR, artificial intelligence, and experimental validation may further accelerate the development of potent and resistance-resilient antimalarial candidates.

Keywords: *Plasmodium* species; Molecular docking; Nitrogen-containing heterocycles; Antimalarial drug discovery; DHFR; Falcipains; Plasmepsins; PfATP4; LDH; PDB ID.

Integrating Network Pharmacology with Experimental Validation to Elucidate the Diuretic Potential of Aqueous Bark Extract of *Ziziphus jujuba*

[1]Mukta Nivrutti Gochade, [2]Dr.Atul Tripathi, [3]Dr. Amol Chandekar
Department of Pharmacy, Konkan Gyanpeeth Rahul Dharkar College of Pharmacy and Research Institute Karjat, Maharashtra, India.
gochademukta@gmail.com

ABSTRACT

Edema, hypertension, and other conditions related to fluid retention are frequently treated with diuretics. But long-term usage of synthetic diuretics can have negative effects, which emphasizes the need for safer substitutes made from plants. Several bioactive phytoconstituents with a variety of pharmacological properties can be found in *Ziziphus jujuba*, which has long been employed in herbal medicine. By combining network pharmacology with experimental pharmacological validation, the current study sought to assess the diuretic capability of *Ziziphus jujuba's* aqueous bark extract. Phytochemical databases and published literature were used to obtain reported phytoconstituents of *Ziziphus jujuba* bark. Protein–protein interaction and pathway enrichment analyses were performed after potential biological targets associated with these phytoconstituents and diuretic activity were found utilizing network pharmacology methods. An established animal model was used to assess the aqueous bark extract's experimental diuretic efficacy. GraphPad Prism was used to examine the measurements of urine volume and electrolyte output. Numerous targets and biochemical pathways linked to renal function, electrolyte balance, and fluid management were found by network pharmacology analysis. The of the experiment showed that, in comparison to the control group, the aqueous bark extract considerably enhanced urine output and electrolyte excretion. By pointing to potential processes behind the diuretic impact, the computational study corroborated the experimental findings. *Ziziphus jujuba's* diuretic potential can be thoroughly investigated by combining network pharmacology with experimental pharmacology. These encourage more research to identify active ingredients and clarify how they work.

Keywords: herbal medicine, network pharmacology, diuretic action, aqueous bark extract, *Ziziphus jujuba*

Contactless Cardio-Respiratory Monitoring Using Millimeter-Wave Radar for Continuous Patient Monitoring

Sai Akash V, Dr. Mohmmad Ashaq Sofi
Department of Biomedical Engineering, School of Bio and Chemical Engineering, Sathyabama Institute of Science and Technology, Chennai-600119
saiakash2432@gmail.com

ABSTRACT

In today's healthcare, ongoing surveillance of vital signs for a short duration is of great importance so that doctors can evaluate the condition of a patient and recognize health problems at an early stage. Usually, doctors monitor patients by attaching sensors and electrodes to the body which might not be appropriate for continuous surveillance. In an effort to address these issues, the research community has been investigating contactless monitoring techniques, especially millimeter-wave radar technology. This work presents the utilization of millimeter-wave radar systems to monitor vital signs such as heart rate and breathing rate. It also considers signal processing techniques, radar system design, and the use of artificial intelligence for higher accuracy and reliability of measurements. Millimeter-wave radar can detect breathing- and heartbeat-induced chest motions without any physical contact with the patient. The analysis indicates that millimeter-wave radar has significant potential for monitoring vital signs in hospitals, at home, in care centres, and for remote patient monitoring. The technology provides a contactless approach for detecting cardiac and respiratory activity. However, important limitations include motion artifacts, high costs of equipment, difficult calculations, and a lack of testing in healthcare settings. Millimeter-wave radar technology shows promising potential for contactless and continuous vital-sign monitoring. Further investigation is required to overcome the existing limitations and to develop reliable, inexpensive, and real-time contactless monitoring systems for healthcare applications.

Keywords: mmWave Radar, Contactless Monitoring, Heart Rate, Respiration Rate, Signal Processing, Health Care.

Role of Inflammatory Biomarkers in the Management of Infectious Skin Diseases

Rajshree Tung, Nimisha[2],
[2]*Professor, Departmet of Pharmaceutics*
Amity Institute of pharmacy,Amity University Uttar Pradesh,Lucknow Campus,Lucknow226028(India) Email-
**rajshree.tung@s.amity.edu,nsrivastava3@lko.amity.edu*

ABSTRACT

Infectious skin diseases represent a significant global health burden often, complicatedbyoverlappingmicrobialinvasionanddysregulatedhostinflammatoryresponses. Conventional diagnostic methods such as cultures and clinical inspection provide limited insight into the dynamic immunological processes underlying infection and healing. Inflammatory biomarkers including cytokines, chemokines and acute-phase reactants offer objective measures of immune activation and tissue damage. Evaluating these biomarkers enhances diagnostic accuracy and provides prognostic information on disease severity, therapeutic response and risk of chronicity. Recent advances in serum biomarker studies and wound immunoprofiling highlight the potential of inflammatory markers as clinical tools to guide management strategies in infectious dermatology. This synthesis integrates evidence from serum biomarker analyses in patient dermatology and multiplex immunoassay profiling of chronic wound swabs. Serum markers such as IL-6, IL-17, ferritin, IgE and procalcitonin were assessed for their diagnostic and prognostic roles. Parallel studies quantified cytokines, chemokines and growth factors in wound samples with emphasison biomarker ratios as predictors of infection and healing status. Pro-inflammatory cytokines (IL-1β, IL-6, IL-17, IL-18) and chemokines (CCL2, CXCL8) consistently elevated in infected or non-healing lesions. Ferritin and CRP/ESR correlated with systemic inflammation while procalcitonin distinguished bacterial from viral etiologies and reflected cellulitis severity. Inflammatory biomarkers provide valuable adjuncts in the management of infectious skin diseases by improving diagnostic precision, guiding antimicrobial therapy and monitoring treatment response. Integration of serum markers with immunomarker profiling offers a promising approach to stratify patients, predict outcomes and personalize interventions.

Keywords: Biomarkers; Dermatological disorders; Disease monitoring; Precision medicine; Therapeutic response

Artificial Intelligence in Pharmacy Practice Aiding Patient-CentredCareand Precision Medicine

Nimisha*
*Professor, Department of Pharmaceutics
Amity Institute of Pharmacy, Amity University Uttar Pradesh, Lucknow Campus, Lucknow 226028 (India)
nsrivastava3@lko.amity.edu

ABSTRACT

The contemporary healthcare ecosystem is undergoing a paradigm shift through the convergence of artificial intelligence (AI), digital health technologies and clinical pharmacy practice. Pharmacists are increasingly positioned to integrate AI-based innovations into precision medicine, therapeutic optimization and patient-centred care. Machine learning (ML), natural language processing (NLP) and predictive analytics enable rapid interpretation of electronic health records, pharmacogenomic datasets and real-world evidence. A narrative literature-based approach was adopted to examine the integration of AI and digital health technologies into contemporary pharmacy practice. Relevant applications of AI, including machine learning, natural language processing, predictive analytics, pharmacogenomics, intelligent clinical decision-support systems, robotic automation and AI- assisted digital platforms were considered. The review focused on their potential roles in clinical pharmacy, hospital pharmacy, community pharmacy, pharmacovigilance, medication therapy management, precision pharmacotherapy and patient-centred care.AI integration into pharmacogenomics enables individualized therapy selection based on genetic markers and drug metabolism pathways supporting reduced toxicity and improved efficacy. Automated signal detection can identify rare or delayed adverse events while robotic automation in drug compounding and inventory management improves operational accuracy and efficiency. Despite its transformative potential AI adoption requires robust data governance, algorithm transparency, patient confidentiality, human oversight and attention to algorithmic bias and accountability. Pharmacy education must incorporate data analytics, informatics and AI ethics.

Keywords: Artificial intelligence; Clinical pharmacy; Digital health; Personalized medicine; Precision medicine, etc.

Translational research on transferosomes for enhanced transdermal delivery of the anti-inflammatory agents

Shankhadip Nandi[1*]
[1]Department of Pharmaceutical Technology, Eminent College of Pharmaceutical Technology, Kolkata - 700126, West Bengal, India
shankhadipnandi@gmail.com

ABSTRACT

Transdermal delivery systems have recently gained attraction in drug administration due to their several benefits over other existing routes. But, the outermost covering of skin acts as a significant barrier for transporting active agents inside the body. Transferosomes are the novel drug delivery systems which are proficient to overcome the different limitations possessed by conventional transdermal delivery systems. They are deformable vesicles consisting lipid bilayer with phospholipids, edge activator and an aqueous core. Transferosomes are usually fabricated by thin film hydration method. They are capable to reach the deeper layers of skin after delivering higher concentrations of active components. Incorporation of edge activators weakens lipid packing to generate vesicular flexibility. Transepidermal osmotic gradients naturally pull the deformable vesicles into deeper regions of the skin. Transferosomes effectively accumulate in inflamed dermal, subcutaneous, or joint tissues while restricting systemic blood plasma fluctuations. They necessitate up to 5-fold lesser topical dosages to generate identical therapeutic outcomes compared to typical commercial preparations. They have the ability for loading a wide range of drugs including proteins, peptides, and vaccines. Transferosomes demonstrated increased bioavailability, regulated drug diffusion, permeation, and enhanced anti-inflammatory activities. Cutting-edge innovations in transferosomes have emerged as a powerful platform to revolutionize transdermal drug delivery systems. On-going research efforts and technological advancements must be continued to address the existing hurdles like formulation intricacy, stability concerns, limited clinical translation, etc. As the pharmaceutical industry moves toward patient-centric, non-invasive delivery platforms, transferosomes discover the path for a new era in transdermal nanomedicine.

Keywords: Transdermal, transferosomes, vesicles, thin film hydration, permeation, anti-inflammatory.

The Green Blueprint against Uterine Fibroids Therapeutic Prospects of *Ceratophyllum Demersum* L.

Sarpavarapu Hemasri, Rapuru Rushendran*, Chitra V*
Department of Pharmacology, SRM College of Pharmacy, Faculty of Medicine and Health Sciences, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District-603203, Tamil Nadu, India
shemasri2005@gmail.com

ABSTRACT

Uterine fibroids (UFs) are the most common benign tumours of the female reproductive tract and represent a major global gynaecological health burden. Global Burden of Disease (GBD) estimates demonstrate their substantial worldwide impact, while the World Health Organization (WHO) emphasizes reproductive health as an essential component of women's well-being. Fibroid progression involves abnormal cellular proliferation, extracellular matrix accumulation, oxidative stress, inflammation, angiogenesis, and hormone-responsive signalling, highlighting the need for safer and fertility-preserving therapeutic approaches.This study investigates the therapeutic prospects of *Ceratophyllumdemersum* L. against UFs using an integrated computational framework incorporating phytochemical profiling, network pharmacology, target prediction, pathway enrichment, molecular docking, and AI-assisted analysis. Reported phytoconstituents were evaluated for their potential interactions with molecular targets and pathways associated with fibroid progression. *Ceratophyllumdemersum* L. contains diverse bioactive constituents, particularly flavonoids, phenolic compounds, and alkaloids, with reported antioxidant, anti-inflammatory, antiproliferative, and cytoprotective properties. Network analysis suggested that these phytochemicals may collectively modulate oxidative stress, extracellular matrix remodelling, apoptosis, angiogenesis, inflammatory signalling, and hormone-responsive pathways. Molecular docking further supported potential interactions between selected constituents and relevant therapeutic targets. *Ceratophyllumdemersum* L. emerges as a promising multitarget phytotherapeutic candidate with potential antifibrotic, antiproliferative, and fertility preserving effects, warranting further experimental validation.

Keywords: Uterine fibroids; *Ceratophyllumdemersum L*; Phytotherapy; Network pharmacology; Molecular docking; Antifibrotic therapy; Precision gynaecology.

Carbon Nanotubes Revolutionizing Drug Delivery System

Srabani Podder*
Department of Pharmaceutics, Eminent College of Pharmaceutical Technology, West Bengal, India
srabani1712@gmail.com

ABSTRACT

The advancement of unique and efficacious delivery systems for drugs is essential for improving pharmacological characteristics of several kinds of therapeutic molecules. Carbon nanotubes (CNTs) have been identified as a novel and highly efficient method for the conveyance and circulation of pharmaceutical agents. CNTs are manufactured by different methods such as Laser ablation method, Arc discharge method, Chemical vapour deposition method. It regularly generates significant interest among scholars owing to its notable properties like surface area, dimensional rigidity, yield strength, and endurance. These attributes can be further adjusted by altering the chirality, diameter, length, and wall properties of CNTs. They are able to encapsulate an array of medicinal substances, like proteins, nucleic acids, and small molecules, offers them an appealing prospect for the modification of drug delivery strategies. Though extremely beneficial, the biocompatibility of CNTs is a serious issue that generates issues over whether they are suitable for targeted delivery of pharmaceuticals. The distinguishing features of carbon nanotubes (CNTs), particularly their heightened surface-to-volume ratios, high aforementioned conductivity and strength, biocompatibility, intuitiveness of modification, and optical features, have spurred their examination as revolutionary carriers for drug and gene delivery. The functional characterisation of carbon nanotubes improves their immunological resistance, biological degradation, biocompatibility, and lowers toxicological effects, thus placing them as promising nanocarriers for alternative therapies. This assessment contains an overview of carbon nanotubes and their prospective use in medication administration, grounded in recent studies.

Keywords: Carbon nanotubes, biocompatibility, targeted drug delivery, nano carrier, surface functionalisation.

In Silico studies of Pyrazole Linked Chalcone Derivatives as potential antibacterial agents targeting dihydrofolate reductase (DHFR) in antibacterial-resistant *Staphylococcus aureus*

Ishu Garg*, Saurabh Kumar Jha, Sayantan Mukhopadhyay
College of Pharmacy, Shivalik Campus, Shimla Bypass Rd, Shiniwala, P.O. Sherpur, Dehradun-248197, Uttarakhand, India
ishupharmaceutics@gmail.com

ABSTRACT

The increasing prevalence of antimicrobial resistance (AMR) arising from trimethoprim-resistant dihydrofolate reductase (DHFR) in *Staphylococcus aureus* has necessitated the development of alternative antibacterial agents. Pyrazole-linked chalcone derivatives have emerged as promising scaffolds owing to their broad-spectrum antimicrobial potential. The present study aimed to computationally evaluate the binding potential of a library of pyrazole-linked chalcone derivatives against both trimethoprim-resistant and wild-type DHFR of *S. aureus*. A combinatorial library of 24 pyrazole-linked chalcone derivatives was designed by varying the substituents at the R1, R2, and R3 positions. The ligands were energy-minimized and subjected to molecular docking against trimethoprim-resistant DHFR (PDB ID 2W9S) and wild-type DHFR (PDB ID 2W9H). The top-performing ligands were subsequently analyzed through structure–activity relationship (SAR), synthetic accessibility (SA), and SwissADME analyses to evaluate their binding characteristics, drug-likeness, and predicted pharmacokinetic properties. Molecular docking identified ten ligands (M12, M14, M17, M18, M19, M20, M21, M22, M23, and M24) with favorable binding affinities toward both DHFR variants. SAR analysis revealed that incorporation of a 4-chlorophenyl substituent at the R3 position enhanced binding affinity by promoting hydrophobic and aromatic interactions, while appropriate electron-withdrawing and electron-donating substituents at the R1 and R2 positions further optimized ligand–protein interactions. SwissADME and SA analyses indicated favorable drug-like characteristics for the selected lead compounds, with M14, M21, and M22 exhibiting the most balanced physicochemical and medicinal chemistry profiles. The integrated computational strategy successfully identified promising pyrazole-linked chalcone derivatives with the potential to inhibit both wild-type and trimethoprim-resistant DHFR of *S. aureus*. The identified lead compounds provide a rational foundation for further synthesis and biological evaluation as potential antibacterial agents against trimethoprim-resistant *S. aureus*.

Keywords: Synthetic accessibility, ADME, Docking, resistant-DHFR, wild-DHFR

CADD in Antifungal Drug Discovery

Pragati Kumari
Geeta Institute of Pharmacy, Geeta University, Panipat, Haryana, India
pragatikri2442@gmail.com

ABSTRACT

Fungal infections are common infectious diseases that can cause serious complications, particularly in immunocompromised individuals. The increasing development of antifungal resistance has created a need for new and effective antifungal agents. Computer-Aided Drug Design (CADD) is a modern computational approach that can accelerate drug discovery by identifying potential drug candidates and predicting their interactions with specific fungal targets. Various CADD techniques, including molecular docking, virtual screening, pharmacophore modeling, QSAR analysis, molecular dynamics simulation, and ADMET prediction, are used to identify and evaluate potential antifungal compounds. Important fungal targets such as (CYP51), β-(1,3)-glucan synthase, and chitin synthase can be investigated to determine the binding affinity and interaction patterns of candidate molecules. CADD approaches facilitate the identification of promising antifungal compounds. Molecular docking helps determine binding affinity and important amino acid interactions, while virtual screening enables the rapid evaluation of large compound libraries. Molecular dynamics and ADMET prediction can further support the stability. CADD provides a valuable, rapid, and cost-effective strategy for antifungal drug discovery. The integration of computational approaches with experimental studies can accelerate lead identification and optimization and may contribute to the development of novel antifungal therapies capable of addressing emerging drug resistance.

Keywords: Computer-Aided Drug Design, Antifungal Drug Discovery, Molecular Docking, Virtual Screening, CYP51, Molecular Dynamics, Antifungal Resistance.

A Network Pharmacological Approach of Asymmetric Curcumin Derivatives to Uncover Multi-Target Mechanism in Prostate Cancer.

Firdous Fatima[1], Lokesh Deb[2], Bharat G. Somkuwar[1], Sushil Kumar Kashaw[3]

1. *Biotechnology Research and Innovation Council-Institute of Bioresources and Sustainable Development - Mizoram (Department of Biotechnology, Government of India), A-1, Nursery Veng, Chawanga Road, Aizawl-796005, Mizoram, India.*

2. Ethnopharmacology Laboratory, BRIC- Institute of Bioresources & Sustainable Development (IBSD) - Regional Centre, 5th Mile, Tadong, Gangtok -737102, Sikkim, India.

3. Integrated Drug Discovery Research Laboratory, Department of Pharmaceutical Sciences, Dr. Harisingh Gour University (A Central University), Sagar-470003, Madhya Pradesh, India.

firdousfatima8298@gmail.com

ABSTRACT

Prostate cancer is ranked 4th worldwide for incidence among all cancers and 8th for cancer mortality in the WHO report, and according to the GLOBOCAN report, prostate cancer is the second most frequently diagnosed cancer globally, with significant changes in both epithelial and stromal cells during initiation and progression of prostate cancer. However, the Wang *et al.* group synthesised asymmetric 1,5-diarylpenta-1,4-dien-3-ones and asymmetric 1,7-diheteroarylhepta-1,4,6-trien-3-one derivatives via the Horner-Wadsworth-Emmons reaction. Furthermore, *in vitro* antiproliferative activity was evaluated in human prostate cancer cell lines (PC-3, DU145, and LNCaP) using both androgen-sensitive and androgen-insensitive cell lines. Consequently, previous studies have highlighted a lack of clarity regarding the single signalling pathway and a specific protein target for antiproliferative activity. Thus, to address this research gap, our study leverages network pharmacology as a robust framework to identify and validate specific protein targets within a defined signalling pathway. By employing computational tools and integrating data from the SwissTargetPrediction and GeneCards databases, we aim to construct comprehensive interaction networks that elucidate potential protein targets of curcumin derivatives to predict the responsible signalling pathway. Furthermore, to find the gene expression data by using the keyword “Prostate Cancer” for the species “Homo sapiens”, a search was performed. A total of 288 common genes were filtered for gene ontology (GO) and protein-protein interaction (PPI) network analyses to identify top hub genes in prostate cancer using Cytoscape. Furthermore, the STRING and DAVID Bioinformatics databases are used to identify molecular functions, biological processes, cellular components, and KEGG pathways in prostate cancer. These hub genes are EGFR, AKT1, KRAS, mTOR, PIK3CA, MMP9, NFKB1, IGF1R, GSK3B, and RAF1. To conclude, our findings suggest that these curcumin derivatives can regulate prostate cancer through specific protein targets.

Keywords: Prostate cancer, Network Pharmacology, Antiproliferative Activity, Gene Ontology (GO), Protein-Protein Interaction (PPI), Hub Genes.

Designing The Future of Pharma Computer-Aided Technologies for Drug & Formulation Innovation

Dr. Niraj Gupta*
Professor, College of Pharmacy Agra, Dr. A.P.J. Abdul Kalam Technical University, Lucknow
nirajg261@gmail.com

ABSTRACT

Computer-Aided Design (CAD) tools have emerged as powerful technologies for accelerating innovation in pharmaceutical sciences. By integrating computational modeling, simulation, visualization, and data-driven approaches, CAD facilitates the rational design and optimization of drug molecules, dosage forms, delivery systems, and pharmaceutical manufacturing processes. This work presents a conceptual review of the application of CAD-based technologies in pharmaceutical research and development. Relevant scientific literature was analyzed to explore the use of molecular modeling, computer-aided drug design (CADD), three-dimensional visualization, computational simulation, and formulation-design software. Their applications in drug discovery, drug–receptor interaction studies, formulation optimization, nanotechnology-based drug delivery, and process development were evaluated. The analysis indicates that CAD tools significantly enhance the efficiency and accuracy of pharmaceutical product development. Molecular modeling supports prediction of drug–target interactions and optimization of lead compounds, while formulation-design software enables systematic evaluation of critical formulation variables. CAD-assisted visualization and simulation further support the development of novel drug delivery systems, including nanoparticles, implants, and controlled-release formulations. Integration with AI and machine learning provides additional opportunities for predictive modeling and rapid decision-making.CAD technologies are transforming pharmaceutical sciences by enabling a more rational, predictive, and cost-effective approach to innovation. Their integration with experimental techniques can minimize development risks and improve product quality and performance. However, challenges such as software cost, data quality, computational requirements, and the need for skilled professionals remain. Overall, CAD represents an important technological platform for advancing modern drug discovery, formulation development, and pharmaceutical manufacturing.

Keywords: Computational Drug Discovery, Digital Formulation Engineering, AI-Integrated Pharmaceutical Design, Next-Generation Pharmaceutical Innovation, Computer-Aided Drug & Delivery Design

Gloriosine as a therapeutic lead for Uterine fibroids A network Pharmacology and *insilico* exploration of Estrogen-progesterone signalling

Ankita Misra*
*Amity Institute of Pharmacy, Amity University Uttar Pradesh, Lucknow Campus, Lucknow-226028, UP, India.
amisra5@lko.amity.edu

ABSTRACT

Uterine fibroids are hormone-responsive benign tumors characterize by excessive proliferation of uterine smooth muscle cells, while estrogen and progesterone signalling playing important roles in their growth and progressions. Gloriosine, an alkaloid of *Gloriosa superba* L., has previously demonstrated promising anti-mitotic and antiproliferative in our previous investigations. Gloriosine showed strong affinity for colchicine binding site of β-tubulin, with a docking score of -7.5 kcal/mol and more than 85% overlap with the binding pattern of colchicine. The molecule exhibits significant antiproliferative activity and showed concentration dependent mitotic inhibition, chromosomal abnormalities and reduced cellular proliferation. With this background, a hypothesis is generated that gloriosine may be promising lead for anti-uterine fibroid (UF) therapy. The study proposes an integrated network pharmacology and molecular docking approach to explore the potential of gloriosine against UF. Putative targets of gloriosine will be mapped with uterine-fibroid-associated genes to identify key molecular targets and signalling pathways, with particular emphasis on estrogen- and progesterone-mediated pathways. Molecular docking will further investigate the interaction gloriosine with key hormonal markers, particularly estrogen receptor (ESR1) and progesterone receptor (PGR), along with prioritized hub target identified through network analysis. The study provides mechanistic basis for further investigation of invitro validation through UF cell model, followed by assessment of cellular proliferation, apoptosis, cell cycle arrest/progression. The study outcomes may establish gloriosine as a potential lead for anti-UF adjuvant therapy.

Keywords: Gloriosine; uterine fibroids; network pharmacology; molecular docking; estrogen receptor; progesterone receptor.

Phytoconstituents Targeting Molecular Biomarkers in Diabetic Dementia Mechanistic Insights and Therapeutic Potential

Anwit Das*, Dr. Komal Patel
Department of Pharmacology, Parul Instituite of Pharmacy, Parul University, Vadodara, Gujarat, India
anwitdas1@gmail.com

ABSTRACT

Diabetic dementia, or multiple neuro-cognitive complications of diabetes, involves insulin resistance, oxidative stress, neuroinflammation, and progressive cognitive dysfunction in the brain. Phytoconstituents are recognized to have multi-target pharmacological properties and hence could offer hope of therapy for the interlinked molecular mechanisms of diabetic dementia. However, the identification of their possible molecular targets is still difficult. In the present work, we put forward an integrated computational pharmacology approach that integrates network pharmacology and molecular docking to identify phytoconstituents that target key molecular biomarkers associated with diabetic dementia. Subsequently, targets for the disease will be retrieved from databases and matched with targets predicted for selected phytoconstituents. Important targets of protein–protein interaction, important targets of pathways will be identified by protein–protein interaction and pathway enrichment analyses. The selected compound–target interaction will then be further assessed by virtual screening (molecular docking) to check for their possible binding affinity and interaction pattern. The proposed approach will likely result in the identification of several phytoconstituent–target interactions that will lead to diabetic dementia by targeting insulin signaling, PI3K/Akt, GSK-3β-mediated tau pathology, oxidative stress, and/or neuroinflammatory pathways. Phytoconstituents with potentially good interactions with the hub targets were expected to be further prioritized using molecular docking. Integration of network pharmacology and molecular docking may provide a systematic and cost-effective strategy for identifying multi-target phytoconstituents with therapeutic potential against diabetic dementia. The computationally prioritized candidates can subsequently be subjected to experimental validation, facilitating mechanism-based natural product drug discovery.

Keywords: Diabetic dementia; Phytoconstituents; Network pharmacology; Molecular docking; Molecular biomarkers; Brain insulin resistance; Computational drug discovery.

Innovations in Intranasal Nanocarrier Drug Delivery: Bridging the GapAcross the Blood–Brain Barrier

Alpana
ABESIT College of Pharmacy, Ghaziabad
alpana.alpu01@gmail.com

ABSTRACT

Nose-to-brain drug delivery has emerged as a promising strategy for enhancing the transport of therapeutic agents to the central nervous system (CNS), particularly for drugs exhibiting poor brain bioavailability and limited permeability across the blood–brain barrier (BBB). This non-invasive approach enables direct drug transport from the nasal cavity to the brain through the olfactory and trigeminal neural pathways, thereby bypassing the BBB and minimizing systemic drug exposure. Consequently, N2B delivery offers rapid onset of action while reducing peripheral adverse effects. Recent advancements in nanotechnology have significantly accelerated the development of intranasal drug delivery systems. A wide range of nanocarriers, including nanoemulsions, microemulsions, polymeric micelles, lipid-based nanoparticles, liposomes, and transfersomes, have been extensively investigated for their ability to improve drug delivery to the brain. These nanoscale carriers enhance the solubility, physicochemical stability, and nasal mucosal permeability of therapeutic molecules, resulting in improved drug absorption and targeted brain delivery. Furthermore, nanocarrier-based systems can overcome several physiological barriers, including the BBB, hepatic first-pass metabolism, and gastrointestinal enzymatic degradation, thereby improving the bioavailability of drugs that are otherwise difficult to administer effectively. In addition, the non-invasive nature of intranasal administration contributes to better patient compliance compared with parenteral routes such as intravenous injection. Equally important are the safety and toxicological considerations associated with repeated intranasal administration of nanocarrier systems, highlighting the need for comprehensive preclinical evaluation and well-designed clinical studies to establish their long-term efficacy and safety. Overall, nanocarrier-assisted nose-to-brain drug delivery represents a transformative platform for the management of central nervous system disorders. By enabling direct, targeted, and efficient drug transport to the brain while reducing systemic exposure, this approach has the potential to overcome the limitations of conventional drug delivery systems and improve therapeutic outcomes for a wide range of neurological diseases.

Keywords: Nanostructure lipid carrier, Blood-Brain Barrier, Nanoparticles, Nanoemulsion, Liposomes, drug targeting.

Computer-Aided Design Tools as Drivers of Innovation in Pharmaceutical Sciences

Farhat Aisha Ansari, Kartik Tiwari[2] and Mohammad Saqlain[2]
[1*]Department of Chemistry, Integral University, Dashauli, Kursi Road, Lucknow, Uttar Pradseh-220026,
[2]Hygia Institute of Pharmaceutical Education & Research, Ghaila Road, Prabandh Nagar, Lucknow, Uttar Pradesh-226020
faisha@iul.ac.in

ABSTRACT

Traditional drug discovery and formulation development are heavily burdened by high clinical attrition rates, astronomical financial investments, and extensive timelines required to bring novel therapeutics from bench to bedside. Modern pharmaceutical research increasingly relies on computational frameworks to streamline this pipeline. Computer-Aided Drug Design (CADD) and associated digital tools offer innovative solutions to overcome physical testing limitations, enabling high-throughput evaluation of massive chemical libraries and intelligent dosage form design. This comprehensive review systematically evaluates primary computational methodologies applied across drug discovery and pharmaceutical technology. Key tools analyzed include Structure-Based Drug Design (SBDD) via molecular docking, Ligand-Based Drug Design (LBDD), and Quantitative Structure-Activity Relationship (QSAR) modeling. Additionally, *in silico* ADMET profiling, molecular dynamics simulations, artificial intelligence algorithms, and specialized software for 3D-printed dosage form design were examined to determine their predictive reliability and operational impact in modern pharmaceutical workflows. The integration of CADD tools significantly enhances lead candidate selection by accurately predicting target binding affinities and metabolic stability prior to wet-lab synthesis. Virtual screening platforms reduce physical compound libraries by up to 90%, drastically lowering experimental costs and synthetic iterations. *In silico* ADMET models reliably identify potential toxicity profiles early in development, reducing late-stage clinical failures. Furthermore, computational modeling in formulation design facilitates the precise optimization of 3D-printed personalized medicines and controlled-release matrices with reproducible pharmacokinetic behavior. Computer-aided design tools represent an indispensable cornerstone of innovation in contemporary pharmaceutical sciences. By merging predictive digital algorithms with experimental pharmaceutics, these tools accelerate candidate selection, optimize complex drug delivery systems, and substantially lower development costs.

Keywords: Computer-Aided Drug Design; Molecular Docking; *In Silico* ADMET; Virtual Screening; 3D-Printed Pharmaceuticals; Quantitative Structure-Activity Relationship

AI-Assisted CADD for Antibiotic Discovery Against MRSA

Vansh Kumar*, Aamir Malik, Neelam Singh
HR Institute of Pharmacy, HRIT University, Ghaziabad
shivangisharma7129@gmail.com

ABSTRACT

Antimicrobial resistance (AMR) is a major global public health challenge that is increasingly compromising the effectiveness of conventional antibacterial therapy. The World Health Organization (WHO) has identified antibiotic-resistant Staphylococcus aureus as a high-priority pathogen, emphasizing the need for continued development of novel antibacterial strategies. Methicillin-resistant Staphylococcus aureus (MRSA) is particularly important because resistance to β-lactam antibiotics is associated with the acquisition of the mecA gene and expression of the low-affinity penicillin-binding protein PBP2a. Targeting PBP2a therefore represents a rational approach for structure-based antibacterial discovery. The present study explores an artificial intelligence-assisted computer-aided drug design (AI-CADD) approach for the preliminary screening of natural phytoconstituents against MRSA PBP2a. Berberine, curcumin and eugenol were selected based on their reported biological and antimicrobial potential, and their chemical structures were obtained from the PubChem database. A verified three-dimensional structure of PBP2a was selected from the Protein Data Bank and used for molecular docking studies with AutoDock Vina/SwissDock. The resulting protein–ligand interactions and docking scores were proposed as criteria for comparative prioritization of the selected compounds. In addition, SwissADME and pkCSM were employed to predict physicochemical, pharmacokinetic and toxicity-related properties. The proposed workflow integrates target-based molecular docking with early drug-likeness and ADMET assessment to identify compounds worthy of further investigation. Such computational approaches can reduce the number of compounds requiring experimental evaluation and facilitate rational lead prioritization. However, docking scores and in-silico ADMET predictions alone cannot establish antibacterial efficacy or safety. The most promising candidates therefore require subsequent experimental validation through microbiological, pharmacological and toxicological studies.

Keywords: Antimicrobial resistance; MRSA; PBP2a; artificial intelligence; computer-aided drugdesign; molecular docking; phytoconstituents; ADMET.

AI-Assisted CADD for Antibiotic Discovery Against MRSA

Shivangi Sharma*, Aamir Malik, Neelam Singh
HR Institute of Pharmacy, HRIT University, Ghaziabad
shivangisharma7129@gmail.com

ABSTRACT

Antimicrobial resistance (AMR) is a major global public health challenge that is increasingly compromising the effectiveness of conventional antibacterial therapy. The World Health Organization (WHO) has identified antibiotic-resistant Staphylococcus aureus as a high-priority pathogen, emphasizing the need for continued development of novel antibacterial strategies. Methicillin-resistant Staphylococcus aureus (MRSA) is particularly important because resistance to β-lactam antibiotics is associated with the acquisition of the mecA gene and expression of the low-affinity penicillin-binding protein PBP2a. Targeting PBP2a therefore represents a rational approach for structure-based antibacterial discovery. The present study explores an artificial intelligence-assisted computer-aided drug design (AI-CADD) approach for the preliminary screening of natural phytoconstituents against MRSA PBP2a. Berberine, curcumin and eugenol were selected based on their reported biological and antimicrobial potential, and their chemical structures were obtained from the PubChem database. A verified three-dimensional structure of PBP2a was selected from the Protein Data Bank and used for molecular docking studies with AutoDock Vina/SwissDock. The resulting protein–ligand interactions and docking scores were proposed as criteria for comparative prioritization of the selected compounds. In addition, SwissADME and pkCSM were employed to predict physicochemical, pharmacokinetic and toxicity-related properties. The proposed workflow integrates target-based molecular docking with early drug-likeness and ADMET assessment to identify compounds worthy of further investigation. Such computational approaches can reduce the number of compounds requiring experimental evaluation and facilitate rational lead prioritization. However, docking scores and in-silico ADMET predictions alone cannot establish antibacterial efficacy or safety. The most promising candidates therefore require subsequent experimental validation through microbiological, pharmacological and toxicological studies.

Keywords: Antimicrobial resistance; MRSA; PBP2a; artificial intelligence; computer-aided drug design; molecular docking; phytoconstituents; ADMET.

Beyond Prediction: Explainable AI in Drug Discovery

Pradeep Yadav*, Ms. Reenu Chauhan
ITS College of Pharmacy, Muradnagar, Uttar Pradesh, India
py586059@gmail.com

ABSTRACT

Artificial intelligence (AI) is becoming an important tool in modern drug discovery because of its ability to analyse large amounts of chemical and biological data and assist researchers in identifying promising drug candidates. AI based approaches are being explored for virtual screening, drug-target interaction prediction, toxicity assessment and lead optimization. However, when an AI model predicts that a particular molecule may be effective, an important question remains: why did the model make that prediction? This lack of transparency is often referred to as the "black-box" problem. Explainable Artificial Intelligence (XAI) offers approaches that can help researchers understand the factors influencing AI predictions. This work presents a literature-based overview of XAI applications in drug discovery, with particular focus on methods such as SHapley Additive exPlanations (SHAP), Local Interpretable Model-Agnostic Explanations (LIME) and other feature-attribution approaches. The reviewed literature suggests that XAI can help identify molecular or biological features associated with individual predictions and allow researchers to compare these findings with chemical properties, structure–activity relationships and existing biological knowledge. Such explanations may support the prioritization of promising candidates and the generation of hypotheses for further investigation. However, XAI explanations depend on the model, dataset and interpretation method and should not be considered proof of a causal mechanism. Experimental validation remains essential. Integrating AI with explainability and scientific validation may therefore provide a more transparent and meaningful approach to AI-assisted drug discovery.

Keywords: Artificial Intelligence; Explainable AI; Drug Discovery; Machine Learning; SHAP; LIME; Drug–Target Interaction; Lead Optimization.

Ai/Ml Guided Design of Antimicrobial Peptides: A Fight Against Antimicrobial Resistance

Abhishek Tyagi*, Abhishek Ghosh, Rikeshwer Prasad Dewangan
Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research, Jamia Hamdard, New Delhi–110062, India
abhishek.jamiahamdard@gmail.com

ABSTRACT

Antimicrobial resistance (AMR) is a major global health concern associated with increasing treatment failure and mortality. The declining efficacy of conventional antibiotics highlights the need for innovative antimicrobial strategies. Antimicrobial peptides (AMPs) are promising alternatives because of their broad-spectrum activity, rapid action and lower propensity for resistance. However, their stability, toxicity and delivery remain important challenges. Artificial intelligence (AI) and machine learning (ML) can accelerate AMP discovery by identifying sequence–structure–activity relationships and predicting desirable peptide properties. The present work explores AI/ML-guided strategies for AMP discovery, prediction and design. AMP databases and genomic, transcriptomic, proteomic and structural datasets were considered for peptide mining. Data mining facilitates the discovery of novel peptide sequences, while computational design can improve antimicrobial activity, stability, specificity and toxicity profiles. Integration of computational screening with experimental validation provides a systematic approach for identifying promising candidates.AI/ML-guided strategies offer an efficient, scalable and promising approach for accelerating AMP discovery and design. Their integration with experimental approaches may help overcome limitations of conventional methods and contribute to the development of next-generation therapeutics against AMR.

Keywords: Antimicrobial Peptides; Antimicrobial Resistance; Machine Learning; Deep Learning; Peptide Design; In Silico; Bioinformatics

Systematic Development and Optimization of Bigel-Based Formulations forEnhanced Topical Drug Delivery

Kajal*, Bhawna Sharma
Dr. K. N. Modi Institute of Pharmaceutical Education and Research, Modinagar
Ghaziabad, Uttar Pradesh, India, 201204
drxkajal1512@gmail.com

ABSTRACT

While the skin offers an attractive route for localized drug delivery, conventional semisolid formulations often struggle with the barrier properties of the stratum corneum, poor skin retention, and uncontrolled drug release. Recently, bigels—innovative biphasic systems combining hydrogel and organogel networks—have emerged as versatile carriers capable of accommodating both hydrophilic and lipophilic drugs within a single platform. However, their therapeutic success relies heavily on precise formulation and processing parameters. This study aims to develop and systematically optimize a bigel-based topical delivery platform. The primary goal is to achieve desirable physicochemical characteristics, improved application properties, and controlled drug release, all while maintaining excellent formulation stability and skin compatibility. The proposed bigel system will be formulated by independently preparing hydrogel and organogel phases, followed by their controlled integration. We will systematically investigate critical formulation variables, including the hydrogel-to organogel ratio, gelling agent types, phase composition, and mixing temperatures. The resulting formulations will undergo comprehensive evaluation for parameters such as pH, viscosity, spreadability, rheological behavior, texture, and physical stability. Finally, *in-vitro* drug release and *ex-vivo* permeation studies will be conducted to map the drug's release mechanism and skin deposition. The major focus of this research goes beyond simply preparing a bigel; it emphasizes establishing a direct structure-property performance relationship. By rationally optimizing the phase ratios and interfacial organization, we anticipate designing a patient-oriented formulation with prolonged skin residence and a finely tuned drug-release profile. Ultimately, this work seeks to strengthen the fundamental understanding of the variables governing bigel architecture and provide a systematic framework for the future design of advanced topical.

Keywords: Bigel; Hydrogel; Organogel; Topical Drug Delivery; Formulation Optimization; Rheology; Controlled Drug Release; Skin Permeation

Geniposide in Rheumatoid Arthritis: Molecular Mechanisms, Multi-Target Pharmacology, and New Directions in Computer-Aided Drug Discovery

Vinayak Singh[1]
KIET School of Pharmacy, KIET Deemed to be University, Ghaziabad, India
*Presenting author: Mr. Vinayak Singh, Student (B-PHARMA 3rd Year),
vinayak.2428bph2746@kiet.edu

ABSTRACT

Rheumatoid arthritis (RA) is a chronic autoimmune inflammatory condition marked by ongoing synovial inflammation, immune system dysfunction, and gradual joint damage. Even with progress in disease-modifying therapies, issues like treatment response, side effects, and drug resistance continue to pose significant challenges, highlighting the need for new multi-target therapeutic approaches. Geniposide, a naturally occurring iridoid glycoside and primary bioactive compound in Gardenia jasminoides, has drawn interest due to its anti-inflammatory, immunomodulatory, and antioxidant effects. This review consolidates published evidence regarding the phytochemistry, pharmacological effects, molecular pathways, and therapeutic significance of geniposide in rheumatoid arthritis and other chronic inflammatory disorders. Special attention is given to experimental RA models, inflammatory signaling pathways, cytokine regulation, pharmacokinetic constraints, and emerging prospects for computer-aided drug discovery. Preclinical evidence suggests that geniposide can lessen arthritis severity, paw swelling, and joint tissue damage, along with lowering levels of pro-inflammatory molecules such as TNF-α IL-1β, IL-6, and IL-17. Reported mechanisms include modulation of NF-κB MAPK, PTEN/PI3 K, and Wnt/β-catenin signaling, indicating a possible polypharmacological mode of action. Recent RA-focused network pharmacology and experimental studies further corroborate its activity against inflammation-related molecular networks. Geniposide represents a promising natural-product scaffold for multi-target RA drug discovery. Integration of molecular docking, polypharmacology, molecular dynamics and ADMET prediction may facilitate identification and optimization of geniposide-derived candidates with improved drug-like properties. Future experimental and clinical studies are required to validate molecular targets, establish safety and determine therapeutic efficacy.

Keywords: Geniposide; Rheumatoid arthritis; Natural product; Anti-inflammatory; Polypharmacology; Molecular docking; CADD; ADMET.

Graph Neural Networks: AI-Driven in Molecular Design

Harsh Vardhan Singh
Maa Gayatri College of Pharmacy, Naini, Prayagraj UP, India
Sharshvardhan014@gmail.com

ABSTRACT

Artificial Intelligence (AI) techniques have recently been increasingly utilized in data-driven healthcare research across various applications, including effective disease diagnosis, therapeutic drug monitoring, precision medicine and research in molecular level regard GNN.Graph neural networks (GNNs) are revolutionizing drug design processes. Over the past GNNs have emerged as transformative tools by accurately modeling molecular structures and interactions with binding targets. Breakthroughs in predicting molecular properties, toxicity assessment, and interaction analysis, along with generative GNNs enhancing virtual screening and novel molecule design, have significantly speed up drug discovery. Then, three representative tasks are proposed based on the three levels of structural information that can be learned by GNNs: node classification, link prediction, and graph generation. Improvements in training time, memory consumption, or reduction in graph sizes using specialized techniques like compact abstraction or edge sampling. Task Performance: Specific improvements in domains like code vulnerability detection, molecular property prediction, or trajectory completion. These GNN driven innovations improve predictive accuracy, cut development costs, and reduce late-stage failures. It focuses on the interdisciplinary integration of GNNs throughout the. discovery process, including lead discovery and optimization, synthetic route design, drug–target interaction prediction, and molecular property profiling, while critically evaluating the challenges in translational medicine.

Keywords: Introduction, applications of GNN, GNN implementation, advancement, advantages and disadvantages, future prospects, conclusion, reference.

3D Printing in Pharmaceutical Formulation Design

Ansh Shukla1
1Department of Pharmacy, Prof. Rajendra Singh (Rajju Bhaiya) University, Naini, Prayagraj, UttarPradesh, India
anshshukla20as@gmail.com

ABSTRACT

Pharmaceutical formulation is changing rapidly with the arrival of three-dimensional (3D) printing, also called additive manufacturing. Traditional tablet-making produces millions of identical tablets from a single mould. 3D printing instead builds each tablet layer by layer using a digital design file. This change means the dose, size, shape, release speed, and even the number of drugs in one tablet can be adjusted for each patient, rather than made the same for everyone. This abstract is based on a review of published research papers, regulatory documents, and case studies collected from sources such as PubMed, ScienceDirect, and PMC, along with official guidelines from the FDA and EMA. The review looks at the history, main printing methods, an important real-world example, and current uses of 3D printing in pharmaceutical formulation from 1986 to 2026. The review shows that this technology began with Stereolithography in 1986, followed by Fused Deposition Modeling in 1992, and Binder Jetting, developed at MIT, in 1993. In 2015, the FDA approved Spritam, the first 3D-printed drug, made using Binder Jetting to create a soft, fast-dissolving tablet for epilepsy, even at high doses. Today, 3D printing is used to create patient-specific doses for children and elderly patients, combine several drugs into one "polypill," design tablets with controlled drug release, and even print medicines directly at hospitals. However, clear rules and regulations for this technology are still being developed around the world. 3D printing is changing pharmaceutical manufacturing from a one-size-fits-all approach to a personalized, made-on-demand approach. While the technology itself is well developed, the lack of clear regulations remains the biggest obstacle to its wider use in hospitals and pharmacies.

Keywords: 3D Printing, Additive Manufacturing, Personalized Medicine, Spritam, Polypill, FusedDeposition Modeling

Editing Life: The CRISPR Revolution

Anas Sayyed and Kaif Hussain
Sanskar College of Pharmacy and Research, Ghaziabad
anasalisayyed556@gmail.com

ABSTRACT

CRISPR is a gene editing technology that uses guideRNA and a Cas9 enzyme to precisely cut and modify DNA. Unlike traditional gene editing methods, CRISPR is a direct, fast, and efficient tool that allows to delete, insert, or correct specific genes. Traditional gene editing tools such as ZFN and TALEN were expensive, complex, and time consuming leading to the development of CRISPR as a cheaper, simpler, and precise method. CRISPR was first introduced in 2014 for the treatment of Duchenne Muscular Dystrophy (DMD) in a mouse model. Following this successful trial, the technology gained wide attention in biomedical research and therapeutic applications. Presently, CRISPR is being widely studied for the treatment of genetic disorders such as sickle cell anemia, cystic fibrosis and cancer gene therapy. It is also being evaluated for viral diseases like HIV and is considered a promising tool in gene therapy. Notably, CRISPR has demonstrated tremendous success in treating DMD and sickle cell anemia while being advanced in other disorders including cancer and HIV. Apart from medicine, CRISPR is used in agriculture for crop improvement, in biotechnology research, animal science and forensic science. Overall, CRISPR is a revolutionary technology with great potential in genetic engineering and future therapeutic applications.

Keywords: CRISPR, gene editing, genetic disorders, cancer therapeutics

Computer Aided Design Tools for Innvation in Pharmaceutical Sciences

Garima Sharma*, Vanshika
Sanskar College of Pharmacy and Research, Ghaziabad, U.P, India
garimasharmanoida18@gmail.com

ABSTRACT

Computer-aided design (CAD) tools have emerged as powerful technologies for accelerating innovation in pharmaceutical sciences by enabling the virtual design, modelling, simulation, and optimization of drugs, formulations, and delivery systems. These computational approaches reduce dependence on conventional trial-and-error methods and facilitate more efficient decision-making during pharmaceutical research and development. In drug discovery, computer-aided drug design (CADD) techniques such as molecular docking, molecular dynamics simulation, pharmacophore modelling, quantitative structure–activity relationship (QSAR) analysis, and virtual screening are widely used to identify potential drug candidates and predict their interactions with biological targets. CAD-based approaches are also increasingly applied in formulation development, including the design and optimization of dosage forms, excipient selection, drug–excipient compatibility, and prediction of drug release profiles. Furthermore, computational modelling can support the development of advanced drug-delivery systems such as nanoparticles, liposomes, and targeted delivery platforms. Integration of CAD with artificial intelligence, machine learning, and three-dimensional modelling has further enhanced the ability to predict pharmaceutical properties and optimize complex development processes. Despite challenges related to computational cost, data quality, model validation, and the need for experimental confirmation, CAD tools offer considerable potential for reducing development time, cost, and failure rates. Thus, the integration of computer-aided technologies with experimental pharmaceutical research represents an important pathway toward faster, more precise, and innovative drug development.

Keywords: Computer-aided design, pharmaceutical sciences, CADD, drug discovery, molecular docking, formulation development, artificial intelligence, drug delivery.

Computer Aided Design Tools for Innvation in Pharmaceutical Sciences

Garima Sharma*, Vanshika
Sanskar College of Pharmacy and Research, Ghaziabad, U.P, India
garimasharmanoida18@gmail.com

ABSTRACT

Computer-aided design (CAD) tools have emerged as powerful technologies for accelerating innovation in pharmaceutical sciences by enabling the virtual design, modelling, simulation, and optimization of drugs, formulations, and delivery systems. These computational approaches reduce dependence on conventional trial-and-error methods and facilitate more efficient decision-making during pharmaceutical research and development. In drug discovery, computer-aided drug design (CADD) techniques such as molecular docking, molecular dynamics simulation, pharmacophore modelling, quantitative structure–activity relationship (QSAR) analysis, and virtual screening are widely used to identify potential drug candidates and predict their interactions with biological targets. CAD-based approaches are also increasingly applied in formulation development, including the design and optimization of dosage forms, excipient selection, drug–excipient compatibility, and prediction of drug release profiles. Furthermore, computational modelling can support the development of advanced drug-delivery systems such as nanoparticles, liposomes, and targeted delivery platforms. Integration of CAD with artificial intelligence, machine learning, and three-dimensional modelling has further enhanced the ability to predict pharmaceutical properties and optimize complex development processes. Despite challenges related to computational cost, data quality, model validation, and the need for experimental confirmation, CAD tools offer considerable potential for reducing development time, cost, and failure rates. Thus, the integration of computer-aided technologies with experimental pharmaceutical research represents an important pathway toward faster, more precise, and innovative drug development.

Keywords: Computer-aided design, pharmaceutical sciences, CADD, drug discovery, molecular docking, formulation development, artificial intelligence, drug delivery.

Self-Medication in the Digital Era: Benefits, Risks and the Influence of Online Health Information

Mayank*, Sakshi Garg

Department of Pharmaceutics, KIET School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh

**mayank.25171042@kiet.edu*

ABSTRACT

Self-medication has emerged as an increasingly common component of healthcare, particularly with the rapid expansion of digital technologies and easy access to health-related information. The availability of over-the-counter medicines, online pharmacies, social media platforms, health websites, mobile applications, and digital communities has made it easier for individuals to identify symptoms and select medicines without professional consultation. Appropriate self-medication for minor and self-limiting conditions may offer advantages such as rapid symptom relief, convenience, reduced healthcare expenditure, and decreased burden on healthcare facilities. However, inappropriate self-medication can result in incorrect diagnosis, inappropriate drug selection and dosage, adverse drug reactions, drug–drug interactions, treatment failure, delayed diagnosis, and dependence or misuse of medicines. The increasing availability of unverified medical information through social media and online platforms further increases the risk of misinformation and irrational medicine use. Self-medication with antimicrobials is of particular concern because inappropriate use can contribute to antimicrobial resistance. Digital health literacy therefore plays an important role in enabling individuals to distinguish reliable medical information from misleading or promotional content. Pharmacists can serve as accessible healthcare professionals by providing evidence-based counselling, identifying potential medication-related problems, promoting rational use of medicines, and referring patients for medical evaluation when necessary. This presentation highlights the evolving pattern of self-medication in the digital era, its potential benefits and risks, factors influencing medicine-use decisions, and strategies for promoting responsible self-care through digital health literacy and pharmacist-led interventions.

Keywords: Self-medication, digital health, antimicrobial resistance, Pharmacist.

Computer Aided Design Tools for Innovation in Pharmaceutical Sciences

Surbhi Jha[1], Palak Tiwari[2], Priyanshi Sharma[3]
Sanskar College of Pharmacy and Research, Ghaziabad, U.P, India
surbhijha67@gmail.com

ABSTRACT

The growing complexity of drug development has created a need for approaches that can efficiently convert scientific information into promising therapeutic solutions. Computer-aided design (CAD) tools have emerged as valuable resources in pharmaceutical sciences by enabling researchers to study, predict, and optimize drug-related properties using computational methods. At the molecular level, computer-aided drug design facilitates the identification of lead compounds through structure-based and ligand-based approaches, including molecular docking, virtual screening, pharmacophore modelling, and quantitative structure–activity relationship (QSAR) analysis. Computational prediction of physicochemical properties and ADMET characteristics further helps researchers assess the suitability of potential candidates during the early stages of development. In pharmaceutical technology, design of experiments (DoE), response surface methodology, and simulation-based tools can assist in optimizing formulation variables, manufacturing conditions, dissolution behaviour, and product quality. Computer modelling is also finding applications in the development of nanocarriers, controlled-release formulations, three-dimensional printed dosage forms, and personalized medicines. More recently, the integration of artificial intelligence and machine learning with conventional computational tools has enabled faster analysis of large pharmaceutical datasets and improved prediction of complex relationships between molecular structure, formulation parameters, and biological activity. Such technologies have the potential to minimize unnecessary experimentation, reduce development time and expenditure, and improve the probability of identifying successful therapeutic candidates. Nevertheless, computational results must be interpreted carefully and supported by appropriate experimental validation. The effective integration of computer-aided tools with laboratory research can therefore provide a multidisciplinary platform for promoting innovation and improving the efficiency of modern pharmaceutical development.

Keywords: Computer-aided design, pharmaceutical sciences, drug discovery, QSAR, molecular docking, design of experiments, formulation optimization, artificial intelligence.

Therapeutic Potential of Quercetin and Eugenol against Arthritis

Sneha Rathore*, Sakshi Garg
Department of Pharmaceutics, KIET School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh
sneharathore853@gmail.com

ABSTRACT

Arthritis, a chronic inflammatory and joint disorder associated with musculoskeletal disorders characterized by degeneration or damage of joints, cartilage degradation, pain stiffness, swelling and restricted movement. Although conventional anti-inflammatory drugs provide symptomatic relief, their prolonged use may be associated with adverse reactions, creating interest in naturally derived bioactive components. Quercetin, a flavonoid/ polyphenolic compound found in onions, apples, berries and several vegetables, possess pharmacological effects including anti-inflammatory, antioxidant, immunomodulatory and bone-protective effects. Preclinical studies indicate that quercetin suppress inflammatory mediators and pathway including NF-κβ, reduce oxidative stress, and can inhibit MAPK pathway including ERK, JNK, p38. Eugenol, a phenylpropanoid phytoconstituent, obtained from clove oil (Syzgiumaromatium) has pharmacological profile. Recent experimental studies have reported that it can reduce inflammatory mediators including TNF-α, IL-6, nitric oxide. Its structure contributes to potent antioxidant potential, while its ability to modulate inflammatory signaling pathways. Quercetin and Eugenol additionally contribute against arthritis inflammation, target multiple pathways involved in arthritis inflammation and oxidative damage. Advanced drug delivery systems such as nanoemulsions or nano-formulations may be explored to overcome poor aqueous solubility and bioavailability limitations associated with quercetin. This review discusses the anti-arthritic potential of quercetin and eugenol, focusing on their molecular mechanisms, antioxidant and anti-inflammatory activities, effects on cartilage and bone metabolism and can be explored to investigate the formulation and evaluation parameters in arthritic gel.

Keywords: Arthritis, Eugenol, Quercetin, anti-inflammatory, NF- κβ, Oxidative stress

Synergistic Anti-halitosis potential of Quercetin and SyzygiumCumini seeds extract

Sweety*, Sakshi Garg
Department of Pharmaceutics, KIET School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh
ss9476047@gmail.com

ABSTRACT

Halitosis (bad breath), a condition affecting oral health and characterized by persistent unpleasant breath odor, associated with generation of volatile Sulphur compound (VSCs) from microbes (bacteria present on tongue and in oral cavity). Although, conventional mouthwashes are available that temporarily control malodor, but their prolonged use is associated with undesirable side effects, therefore, a need to formulate a safe and effective natural alternative. Quercetin, a natural bioactive ingredient possesses antibacterial and antioxidant properties while Syzygiumcumini (Jamun) seeds are rich in phenolic compounds, tannins and flavonoids. They work by inhibiting the growth of oral bacteria and reduction of volatile sulphur compound (H_2S). Pharmacological potential of these agents enhanced activity and inhibit oral microorganisms involved in plaque formation and periodontal inflammation. This review explores the synergistic anti-halitosis potential of quercetin and *S. cumini* seed extract, with emphasis on inhibition of halitosis-associated oral microorganisms. This combination may exert its effects through multiple mechanisms, including disruption of microbial cell membranes, modulation of inflammatory pathways, inhibition of microbial enzymes, reduction of oxidative stress, and interference with biofilm development. Quercetin and Jamun seeds extract may be used in synergestic approach to improve bad breath and reduce by formulating into a suitable dosage form including mouth wash and mouth freshner.

Keywords: Halitosis, Quercetin, Anti-inflammatory, Periodontal inflammation, Syzygiumcumini

Plant-Derived Bioactive Compounds as Emerging Therapeutic Leads: Molecular Docking Insights into Drug–Target Interactions

Mr. Sujal*, Mrs. Khushboo Bansal
Affiliation: Sunder Deep Pharmacy College, SDGI Global University
Sujalguru9918@gmail.com

ABSTRACT

The discovery and development of novel therapeutic agents remain major challenges in modern pharmaceutical research due to increasing drug resistance, adverse effects, high development costs, and the prolonged timeline associated with conventional drug discovery. Phytochemicals, naturally occurring bioactive constituents derived from medicinal plants, represent a valuable and structurally diverse source of potential drug candidates. Compounds such as alkaloids, flavonoids, terpenoids, phenolics, tannins, and glycosides have demonstrated diverse pharmacological activities, including antioxidant, anti-inflammatory, antimicrobial, anticancer, antidiabetic, and neuroprotective effects. However, the identification and optimization of bioactive phytochemicals through conventional experimental approaches can be laborious and time-consuming. Molecular docking has emerged as a potent computational tool for forecasting the interaction of phytochemicals with a biological target at the molecular scale. It is a technique that is utilized for the swift screening and selection of promising phytoconstituents by estimating the binding affinity, ligand binding configuration, and key ligand-target interactions prior to experimental validation. Phytochemical profiling along with molecular docking, molecular dynamics simulations, pharmacological efficiency of bioactive molecules and other computational approaches can offer a holistic understanding of the mechanisms underlying the therapeutic potential of plant-derived compounds. This integrated strategy may accelerate lead identification, reduce research costs, and support the rational design and optimization of novel drugs. Computational predictions require appropriate validation through in vitro, in vivo, pharmacokinetic, toxicological, as well as clinical studies. Thus, the integration of phytochemistry and molecular docking represents a promising and futuristic approach for discovering more selective, safely and potentially effective therapeutic agents from natural bioactive compounds.

Keywords: - molecular docking, drug discovery, ligand–target, pharmacokinetic, toxicological, rational design, bioactive compounds

Drug Information Database: A Vital Tool for the Modern Pharmacist

Richa Yadav, Khushboo Bansal*
Department of Pharmaceutics, Sunderdeep Pharmacy College, Dasna, Uttar Pradesh, India
ry353997@gmail.com

ABSTRACT

The growing complexity of new medicines and therapies makes the management of healthcare data difficult to handle, calling for the development of advanced computer tools for pharmacists' safe practice. Drug information databases represent an excellent virtual platform for clinical pharmacy, offering the pharmacist the possibility to consult the right drug profile prior to dispensing or giving advice in a real-world setting. With the help of electronic screening tools, pharmacists can rapidly explore and sort out extensive lists of medications depending on the target health issue. The best candidates from the database lists can be subjected to electronic safety checks on the computer screen, predicting the actual risk of different physical interactions of the selected drugs by reviewing clinical alerts, including negative drug to drug interactions, duplicate therapies, safely on a computer screen. In addition, combination of Artificial Intelligence (AI) with virtual medical databases can support the identification of the safest options for medication by interpreting the likelihood that a specific dose of a drug may match the age and personal metabolism of the recipient and the risk of toxic side effects at the initiation of therapy. Thus, though such computer-based drug screenings require complex considerations such as modern clinical practice guidelines and data accuracy. Therefore, the use of drug databases along with the electronic screening tools, safety alerts, and the presence of artificial intelligence and clinical double-checking represent an excellent approach to hasten modern pharmacists' practice, eliminating dangerous uncertainties in the drug distribution process from the prescription to the healthy patient.

Keywords: Drug Information Database; Pharmacist Tools; Clinical Pharmacy; Artificial Intelligence; Drug Interactions; Patient Safety; Medication Management; Healthcare Technology.

Rational Design, In Silico Profiling, Synthesis and Biological Evaluation of Novel Chalcone-Based Derivatives: An Integrated Drug Discovery Approach

Saurabh Singh[1]*, Manish Kumar Pathak[1]

[1]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Swami Vivekanand Subharti University, Meerut (U.P.), India – 250005

sssaurabhsingh8279@gmail.com

ABSTRACT

Chalcone is a simple yet versatile scaffold that has attracted considerable attention in medicinal chemistry because of its α, β-unsaturated carbonyl group and its ability to support diverse biological activities. The present work was undertaken to explore chalcone derivatives through a combined computational, synthetic, and biological approach. A focused series of substituted chalcone derivatives was designed by varying the substituents on the aromatic rings to examine their influence on molecular interactions and biological performance. The designed compounds were subjected to in silico evaluation, including molecular docking, to assess their binding orientation and interaction with selected therapeutic targets. Compounds showing favourable computational profiles were selected for synthesis using the Claisen–Schmidt condensation reaction. The synthesized derivatives were characterized by FT-IR, NMR, and mass spectrometric techniques. Their biological potential was assessed using selected in vitro assays. Computational screening indicated that structural substitution on the aromatic rings influenced the predicted binding pattern and interaction profile of the chalcone derivatives. The synthesized compounds showed characteristic spectral features consistent with the proposed structures. Initial biological evaluation demonstrated differences in activity among the derivatives, suggesting that the type and position of substituents contribute to the observed biological response. The combined computational and experimental findings also provided useful indications for preliminary structure–activity relationship analysis. The study demonstrates that integrating rational design, in silico profiling, chemical synthesis, and biological testing can provide a practical route for identifying promising chalcone-based molecules. The findings support further optimization of selected derivatives and their detailed mechanistic and in vivo investigation as potential therapeutic leads.

Keywords: Chalcone derivatives, Rational drug design, Molecular docking, In silico profiling, Claisen–Schmidt condensation, Structure–activity relationship, biological evaluation, Medicinal chemistry.

Engineering Pickering Nanoemulsions for Enhanced Delivery of BCS Class III Drugs: A Novel Approach to Improving Oral Drug Performance

Siddharth Dhaka[1]*, Sumita Singh[1]

[1]Department of Pharmaceutics, Faculty of Pharmacy, Swami Vivekanand Subharti University, Meerut (U.P.), India – 250005

siddharthdhaka54@gmail.com

ABSTRACT

Oral delivery of BCS Class III drugs remains challenging because, despite their favourable aqueous solubility, their limited intestinal permeability can result in inadequate and variable drug absorption. Pickering nanoemulsions, stabilized by finely dispersed solid particles at the oil–water interface, offer an interesting platform for modifying drug release and improving the performance of orally administered drugs. The present study aimed to develop and evaluate a Pickering nanoemulsion-based delivery system for a selected BCS Class III drug. The formulation was designed by selecting suitable oil, aqueous, and particulate stabilizing components based on their compatibility with the drug and their ability to form a stable nanoemulsion. Formulation variables were systematically optimized to obtain desirable droplet characteristics and physical stability. The developed formulations were evaluated for appearance, pH, droplet size, polydispersity index, zeta potential, drug content, entrapment efficiency, and storage stability. In vitro drug-release behaviour was also investigated and compared with the conventional drug formulation to assess the potential of the developed system. The optimized Pickering nanoemulsion exhibited nanoscale droplets with a comparatively uniform distribution and satisfactory physical stability. The formulation demonstrated consistent drug incorporation and showed improved in vitro drug-release behaviour compared with the conventional drug system. The presence of a particle-stabilized interfacial layer appeared to contribute to the stability of the formulation and controlled interaction of the drug-loaded droplets with the aqueous environment. The developed Pickering nanoemulsion represents a promising approach for improving the delivery characteristics of BCS Class III drugs. This strategy may provide a useful formulation platform for overcoming permeability-related limitations and warrants further investigation through permeability studies and in vivo pharmacokinetic evaluation.

Keywords: Pickering nanoemulsion, BCS Class III drugs, Drug delivery, Nanoformulation, Oral drug delivery, Permeability enhancement, Formulation development, pharmaceutical nanotechnology.

Evaluation of Antiepileptic and Neuroprotective efficacy of a Selected Medicinal Plant leaf extract in Mice

Drishti Srivastava1*, Ms. Monika Singh2

1Research Scholar, Department of Pharmacology, I.T.S College of Pharmacy, Ghaziabad, India,

2Associate Professor, Department of Pharmacology, I.T.S College of Pharmacy, Ghaziabad, India

Drishtisrivastava2310@gmail.com

ABSTRACT

Recurrent epileptic seizures stimulate cascades of neuropathological destruction, primarily driven by glutamate-mediated excitotoxicity, severe intracellular oxidative stress, and progressive neurodegeneration. While traditional antiepileptic therapies suppress hypersynchronous electrical discharges, they fail to arrest underlying brain tissue damage, hippocampal cell loss, and cognitive decline. Natural plant therapeutics possess complex multi-target secondary metabolites capable of penetrating the blood-brain barrier to target convergent necrotic and apoptotic cascades, offering substantial neuroprotective shielding and structural preservation alongside core anticonvulsant activity. Crucial clinical parameters—including seizure latency, behavioral severity grading, and overall survival rates—will be tracked. Advanced post-seizure tissue analysis will be performed on brain homogenates to determine neuroprotective integrity, focusing on targeted biomarker assays for oxidative stress (malondialdehyde, reduced glutathione, superoxide dismutase) and structural neurotransmitter restoration frameworks.This pharmacological investigation is anticipated to validate that the selected medicinal plant leaf extract serves as a robust neuroprotective framework capable of attenuating seizure-induced cellular injury and promoting brain tissue survival. These concrete findings will provide a critical preclinical reference to support subsequent isolation, characterization, and downstream synthesis compounds for advanced neuroprotection and holistic management of epilepsy.

Keywords: Neuroprotection, Seizure-Induced Neurodegeneration, Excitotoxicity, Antiepileptic, Oxidative Stress, Selected Medicinal Plant

Mechanistic Evaluation of the Antiepileptic and Neuroprotective Effects of a Selected Medicinal Plant in Experimental Animal Model

Manish[1*], Monika Singh[2]
[1*]Research Scholar, Department of Pharmacology, I.T.S College of Pharmacy Ghaziabad, India,
[2]Associate Professor, Department of Pharmacology, I.T.S College of Pharmacy Ghaziabad, India,
msarurpur@gmail.com

ABSTRACT

Epilepsy is associated with abnormal neuronal excitability and recurrent seizures resulting from an imbalance between excitatory and inhibitory neurotransmission. Natural products have attracted considerable attention because of their diverse phytochemical composition and potential ability to modulate multiple pathways involved in seizure generation.The present investigation aims to evaluate the antiepileptic activity of a selected medicinal plant leaf extract in experimental animal models and to explore the possible mechanisms underlying its anticonvulsant and neuroprotective effects.The selected leaves will be extracted using an appropriate solvent system and subjected to qualitative phytochemical evaluation. The pharmacological activity of the extract will be assessed in validated animal models of chemically induced seizures. Seizure latency, severity, duration, protection against convulsions, and survival will be recorded. Depending upon the experimental design, biochemical investigations involving oxidative stress markers and neurotransmitter-related parameters may be performed to determine whether the observed activity is associated with antioxidant protection and modulation of neuronal excitability. The study may establish the potential of the selected medicinal plant as a source of anticonvulsant and neuroprotective phytoconstituents. Positive findings could provide a scientific basis for further isolation, characterization, and mechanistic evaluation of its active constituents for potential application in epilepsy management.

Keywords: Seizure, Anticonvulsant, Neuroprotective, Epilepsy, Neurotransmitter

Drug Discovery and Development by using the Tech: Artificial Intelligence

Manmohan Singh*, Manish Kumar Kaushik
HR Institute of Pharmacy, HRIT University, Ghaziabad
manmohan.prajapat2005@gmail.com

ABSTRACT

Artificial Intelligence (AI) uses computational algorithms to analyze complex biological and chemical data. In modern pharmaceutical research, AI can help researchers identify drug targets and promising molecules. It can also accelerate important stages of drug discovery, such as drug design, virtual screening, and ADMET prediction. Therefore, AI can potentially reduce the time and cost of early drug discovery. The first step is Target Identification. A drug target is a specific biological molecule, usually a protein, receptor, or enzyme, that is involved in a disease process. There is a large amount of genomic, proteomic, and biological data available to researchers. AI can analyze this complex data and help identify potential disease-related targets. It can also predict drug-target interactions and help researchers prioritize the most promising targets for further drug development. Once the target is identified, the next step is AI-Based Drug Design. AI uses computational models to design and optimize molecules that can interact with the selected drug target. It can predict suitable drug molecules and generate or suggest potential molecules. AI can also optimize these molecules for better binding and activity. This process helps researchers identify promising drug candidates. The next stage is Virtual Screening. Virtual screening is a computational method used to evaluate a large number of molecules. AI can screen large molecular libraries and predict how different molecules may interact with the selected target. It can rank the molecules according to their predicted binding and select the most promising molecules for further testing. After virtual screening, the promising molecules undergo ADMET Prediction. ADMET stands for Absorption, Distribution, Metabolism, Excretion, and Toxicity. However, AI-driven drug discovery also has some challenges. These include limited availability of high-quality biological and chemical data, possible errors or bias in AI predictions, and the need for experimental validation. Also, complex biological systems can be difficult to model accurately. Looking at the future scope, more accurate AI models may improve drug discovery. AI can also be integrated with genomics and personalized medicine. It may help in faster identification of novel drug candidates and improve the prediction of drug efficacy, safety, and toxicity. To conclude, AI is becoming an important computational tool in modern drug discovery. It can support researchers at different stages, from target identification to the selection of promising drug candidates.

Keywords: Drug target, Experimental validation, Target Identification, Virtual Screening

Machine Learning with Artificial Intelligence and its use in Pharmacy

Yash Katyan*, Piyush Mangla, Manish Kaushik
HR Institute of Pharmacy, HRIT University, Ghaziabad
mr.scenarioman@gmail.com

ABSTRACT

Artificial Intelligence enables computers to perform tasks that normally require human intelligence, such as learning, reasoning, and decision-making. Data science collects, processes, and analyzes data to find useful patterns and insights for better decisions. Machine learning helps computers learn from data, find patterns, and make predictions. In pharmacy, data can include drug properties, patient information, drug dose, and laboratory results. There are three main types of machine learning. Supervised learning learns from data where the correct answer is already known. For example, we give a computer information about 1,000 drugs and also tell it which drugs are safe and which are toxic. It studies the information and finds patterns. Later, when we give information about a new drug, it can predict whether the drug is more likely to be safe or toxic. Second is unsupervised learning. Here, we do not provide correct answers. The computer finds hidden patterns, relationships, and groups by itself. For example, it can study patient data and group patients according to similar medicine responses, age, or health conditions. Reinforcement Learning is when a computer learns by trial and error. It receives a reward for correct actions and a penalty for wrong actions, gradually learning the best decision. Machine learning can support drug discovery, drug formulation, manufacturing, and clinical pharmacy. It uses features (inputs) such as age, weight, drug dose, kidney and liver condition to predict a label (outcome), like whether a patient may have an adverse drug reaction. Data is usually split into training data (80%) to teach patterns and testing data (20%) to check new, unseen performance. Good models avoid overfitting and underfitting by balancing bias and variance. The process includes defining the problem, collecting and cleaning data, selecting features, splitting data, training, evaluating, and predicting. In pharmacy, ML supports drug discovery, formulation, manufacturing, pharmacovigilance, clinical pharmacy, and personalized medicine.

Keywords: Drug discovery, Pharmacovigilance, Machine learning, Data science, Bias, Variance

Machine Learning-Based Prediction of ADMET Properties for Early Drug Candidate Screening

Yashvardhan Sharma[1], Shubhanshu Goel[1]*, Gaurav Chaudhary[1]
[1]I.T.S College of Pharmacy, Ghaziabad, 201206, India
shubhanshugoel06@gmail.com

ABSTRACT

The development of a successful drug candidate requires adequate efficacy as well as favorable pharmacokinetic and safety characteristics. A major proportion of drug candidates are discontinued during development because of undesirable absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties. Consequently, early assessment of ADMET characteristics is essential for reducing late-stage failures and improving the efficiency of drug discovery. Machine learning (ML) has emerged as a powerful computational approach for predicting ADMET behavior from molecular structure and experimental data. ML models can analyze complex relationships between molecular descriptors, fingerprints, physicochemical characteristics, and biological responses to estimate important properties such as intestinal absorption, aqueous solubility, plasma protein binding, blood–brain barrier permeability, metabolic stability, cytochrome P450 interactions, and potential toxicity. Algorithms including random forest, support vector machines, gradient boosting, and artificial neural networks have demonstrated utility in virtual screening and compound prioritization. More recently, deep learning and graph-based approaches have enabled models to directly capture structural information from molecular graphs, potentially improving prediction of complex drug-related properties. Despite these advantages, reliable ADMET prediction remains dependent on high-quality and sufficiently diverse datasets. Data imbalance, experimental variability, limited model interpretability, and restricted applicability to chemically novel compounds can affect predictive performance. Therefore, computational predictions should complement rather than completely replace laboratory-based evaluation. Integrating ML-based ADMET prediction with molecular modeling, in vitro assays, and subsequent experimental validation can facilitate the identification of safer and more promising candidates at an early stage. Overall, ML-assisted ADMET screening provides a data-driven strategy for reducing unnecessary experimental testing, accelerating candidate selection, and supporting more efficient drug development.

Keywords: Machine learning; ADMET; Drug discovery; Virtual screening; Pharmacokinetics; Toxicity prediction; Molecular descriptors; Deep learning; Drug candidate screening.

AI-Based Optimization of Transdermal Drug Delivery Systems

Umang Aggarwal[1], Dr. Madhu Verma[1*]
[1]I.T.S College of Pharmacy, Ghaziabad, 201206, India
madhuverma@its.edu.in

ABSTRACT

Transdermal drug delivery systems provide an attractive alternative to conventional oral and parenteral administration by enabling drug transport across the skin and potentially maintaining prolonged therapeutic exposure. However, the development of an effective transdermal formulation is challenging because skin permeability, drug physicochemical characteristics, formulation composition, and processing conditions can interact in complex ways. Artificial intelligence (AI) and machine learning (ML) techniques are increasingly being explored to address these challenges by supporting formulation prediction, optimization, and performance assessment. AI-based models can analyze relationships between formulation variables and critical quality attributes, including drug release, permeation rate, flux, lag time, adhesion, and formulation stability. Input parameters may include drug molecular properties, polymer type and concentration, penetration enhancers, lipid components, patch thickness, preparation conditions, and physicochemical characteristics. Algorithms such as artificial neural networks, random forest, support vector regression, and gradient-boosting methods can be used to identify influential variables and predict formulation outcomes. AI can also facilitate systematic selection of formulation compositions, reducing the number of experimental trials required during development. Integration of AI with design of experiments, molecular modeling, imaging techniques, and in vitro skin permeation studies may further strengthen formulation development and enable more precise optimization. Despite these advantages, limitations related to data availability, dataset quality, model interpretability, external validation, and differences between experimental and clinical conditions remain important considerations. Future development should emphasize standardized datasets, explainable AI, robust validation, and integration with experimental evidence. Overall, AI-assisted optimization has considerable potential to accelerate the development of reliable, patient-oriented transdermal drug delivery systems while reducing development time and experimental resource requirements.

Keywords: Artificial intelligence; Machine learning; Transdermal drug delivery; Formulation optimization; Skin permeation; Drug release; Predictive modeling; Pharmaceutical development.

Artificial Intelligence in 3D-Printed Personalized Drug Delivery System

Aryendu[1], Shubhanshu Goel[1]*, Gaurav Chaudhary[1]
[1]I.T.S College of Pharmacy, Ghaziabad, 201206, India
shubhanshugoel06@gmail.com

ABSTRACT

Personalized drug delivery aims to provide medicines that are tailored to the individual requirements of patients by considering factors such as dose, release profile, treatment duration, and therapeutic needs. Three-dimensional (3D) printing has emerged as an innovative pharmaceutical manufacturing technology capable of producing drug delivery systems with customized geometries, drug loading, and release characteristics. However, selecting appropriate printing parameters and formulation variables can be challenging because multiple factors may simultaneously influence the quality and performance of the final dosage form. Artificial intelligence (AI) offers a promising computational approach for addressing these challenges by analyzing complex relationships between formulation composition, printing conditions, material properties, and drug release behavior. Machine learning algorithms can be trained using experimental data to predict critical quality attributes, including drug content, mechanical properties, dissolution rate, porosity, printing accuracy, and release kinetics. AI can also assist in optimizing parameters such as extrusion temperature, printing speed, infill density, layer height, nozzle characteristics, and polymer concentration. Combining AI with 3D printing may enable rapid development of patient-specific tablets, implants, films, and other advanced dosage forms with controlled or programmable drug release. Furthermore, predictive models can reduce experimental trials, improve process efficiency, and support quality-by-design approaches. Despite these advantages, challenges involving limited datasets, variability in printing processes, model interpretability, data standardization, regulatory requirements, and reproducibility must be addressed before widespread implementation. Integration of AI with experimental validation and advanced pharmaceutical manufacturing technologies could establish a more flexible and data-driven framework for personalized medicine. Overall, AI-assisted 3D printing represents a promising strategy for developing customized drug delivery systems and advancing patient-centered pharmaceutical therapy.

Keywords: Artificial intelligence; 3D printing; Personalized drug delivery; Machine learning; Pharmaceutical manufacturing; Customized dosage forms; Drug release; Patient-specific therapy; Additive manufacturing.

Molecular Docking and In Silico ADME Evaluation of Curcumin, Quercetin, and Resveratrol against Key Targets in Oral Squamous Cell Carcinoma

Makrani Shaharukh Ismail [1*], Noorul Hasan[2]
[1]Department of Pharmaceutics, Faculty of Pharmacy, Maulana Azad University, Jodhpur, Rajasthan, India
[2]Department of Pharmacology, Faculty of Pharmacy, Maulana Azad University, Jodhpur, Rajasthan, India
makranishaharukh@gmail.com

ABSTRACT

Oral squamous cell carcinoma (OSCC) is one of the most common malignancies of the oral cavity connected with poor outcomes, mainly in advanced disease. The examination for safer and multitarget therapeutic approaches has therefore encouraged interest in naturally occurring phytochemicals such as curcumin, quercetin, and resveratrol.The present study aimed to evaluate the molecular interactions of curcumin, quercetin, and resveratrol with two cancer-related targets, CDK4/Cyclin D1 and the PI3Kα Ras-binding domain, using molecular docking and in silico ADME analysis.The crystal structures of CDK4/Cyclin D1 (PDB ID 2W9F) and the PI3Kα Ras-binding domain (PDB ID 6VO7) were obtained from the Protein Data Bank. Protein structures were prepared using Schrödinger Maestro, while ligand structures retrieved from PubChem were prepared using LigPrep with the OPLS2005 force field. Molecular docking was performed using the Glide Extra Precision (XP) protocol. The resulting docking scores and protein–ligand interactions, including hydrogen bonds, hydrophobic contacts, and polar interactions, were examined. Predicted pharmacokinetic and drug-likeness properties were assessed using QikProp.Curcumin showed the most favourable Glide XP docking score with CDK4/Cyclin D1 (−4.1572 kcal/mol), while quercetin showed the most favourable score with PI3Kα (−4.8846 kcal/mol). Resveratrol also demonstrated favourable interactions with both targets. The in silico ADME assessment indicated generally acceptable predicted pharmacokinetic and drug-likeness characteristics for the three phytochemicals. The docking indicate that curcumin, quercetin, and resveratrol can interact with key molecular targets associated with OSCC. Curcumin showed a favourable interaction with CDK4/Cyclin D1, whereas quercetin demonstrated a comparatively stronger docking score against PI3Kα. These findings support further computational and experimental investigation of these phytochemicals as potential leads for OSCC drug discovery.

Keywords: Oral squamous cell carcinoma; Curcumin; Quercetin; Resveratrol; Molecular docking; CDK4/Cyclin D1; PI3Kα; In silico ADME.

AI-Driven Drug Repurposing for Emerging Diseases Current Trends, Challenges and Future Perspectives

Deepanshu Rathi* Mr. Shardendu Mishra
KIET School of Pharmacy, KIET Group of Institutions, Delhi-NCR, Ghaziabad 201206, UP, India
deepanshu.2425bpharm@kiet.edu

ABSTRACT

Emerging and re-emerging diseases have become major global health issues caused by several factors, including the emergence of new pathogens, antimicrobial resistance and population growth. For the development of new medicines is complex, time-consuming and requires significant resources. Drug repurposing uses existing, approved drugs for new diseases or new therapeutic indications. Relevant research and review articles on AI-based drug repurposing and emerging diseases were collected. Relevant articles were identified using Keywords: such as AI, drug repurposing, Machine Learning, Deep Learning etc. Important information was extracted from the relevant articles and then analyses to understand how AI is used in drug repurposing. The main AI applications, current trends and challenges were compared and studied. By reviewing the literature, it is known that AI/ML can help identify existing drugs that may be beneficial for treating new or emerging diseases. AI can analysis large amounts of biomedical data at once. For emerging diseases such as COVID-19, mpox, Zika, and Ebola, AI-based drug repurposing approaches have been investigated to identify potential drug candidates more quickly. However, there are also some major problems, such as biased data, black-box models, lack of validation, and privacy and regulatory issues. Overall, AI-driven drug repurposing is a promising approach that can accelerate the process of identifying treatments for emerging diseases. Predicted Drugs must be validated through in-vitro testing, followed by in-vivo testing, and clinical trials. In the future, integrating Explainable AI, Generative AI, and precision medicine could make AI-based drug repurposing more accurate, reliable, and clinically useful.

Keywords: Artificial Intelligence, Drug Repurposing, Machine Learning, Deep Learning, Emerging Diseases.

Computational Screening of Herbal Phytoconstituents for Targeted Modulation of Dermal Matrix Degradation in Striae Distensae

Dr. Nandini Girish[1], Darshan Mutgekar[2], Neha Vinod Nirbhavane[3], Rutuja Ravindra Kumawat[4]
Department of Bioanalytical Sciences, Ramnarain Ruia Autonomous College, Mumbai, India
nandinigirish@ruiacollege.edu

ABSTRACT

Striae distensae (SD), commonly known as stretch marks, are dermal lesions characterized by extracellular matrix (ECM) disruption driven by rapid tissue expansion, mechanical strain, and hormonal shifts. Collagen and elastin form the structural backbone of the dermal ECM, whereas elevated activity of matrix metalloproteinases (MMPs), collagenase, and elastase accelerates ECM breakdown, compromising dermal architecture. This study uses a computationally guided approach to evaluate the therapeutic potential of apigenin and β-asarone in preserving dermal matrix integrity. The proposed approach evaluates apigenin and β-asarone as representative phytoconstituents for computational investigation. Three-dimensional structures of selected protein targets associated with ECM degradation were prepared, followed by molecular docking of the selected phytoconstituents. Docking scores, predicted binding affinity, binding orientation, interacting amino-acid residues and non-covalent interactions, including hydrogen bonding and hydrophobic interactions, were considered for evaluating phytoconstituent–protein interactions. The computational investigation is expected to identify potentially favourable interactions of apigenin and β-asarone with selected MMPs, collagenase and elastase targets. Such predicted interactions may provide a molecular basis for investigating whether these phytoconstituents can potentially modulate excessive degradation of collagen and elastin. The findings may also help prioritize promising phytoconstituents and protein targets for subsequent experimental validation. The study integrates herbal formulation development with molecular docking to establish a mechanistic basis for a proposed herbal formulation targeting dermal matrix degradation. Computational findings can guide future enzyme inhibition studies, phytochemical standardization, dose optimization, formulation development and biological validation.

Keywords: Striae distensae, Apigenin, β-asarone, Molecular docking, MMPs, Collagenase; Elastase, Extracellular matrix, Herbal formulation, In silico drug discovery.

Dual carrier system as novel delivery platform for poorly permeable drugs under BCS class III category

Nikhil Kumar*, Anoop Kumar
Dr KN Modi Institute of Pharmaceutical Education and Research, Modinagar, Ghaziabad
nikhil.prajapati741726@gmail.com

ABSTRACT

Poorly permeability across intestinal membrane is major concern affecting oral bioavailability of drugs especially BCS class III drug. Drug can be traversed followed by distinct mechanism viz. active transport, ion pair, or mediated through pore or lymphatics. Several other pathways followed by the drug during transit process like endocytosis, receptor mediated transport, p-glycoprotein inhibition and CYP metabolism. Interplay of physiochemical properties viz. drug polarity, its lipophilic character and ionization constant, are key determinants associated with permeability. It can be modulated through formation of different frameworks whereby hydrophilic character of drug was transformed via ion-pair complexes, phospholipid complexation, or bile salt adducts or with physically interacted with surfactant. But, complexity of the system and its rationale of design is questionable. Most of these approaches are hydrophobically modified ones, and needs lipid-based nano-dispersions Lipid based nanocarriers such as SNEEDS, nano particles, liposome, solid lipid nano particles can accommodate these modifications with enormous surface area and lipophilic microenvironment at absorption cell. Such dual systems can cargo hydrophilic or low lipophilic drug which can manipulate the drug permeability. Self-Nanoemulsifying Drug Delivery System (SNEDDS) is isotropic mixture of oil, surfactant and co-surfactant to form fine nano-emulsion which lead to enhance the interfacial surface area. Solid lipid nanoparticles are fabricated from solid lipid matrix was nanosized to overcome instability, cargo drug in surfactant and manipulate drug permeability. Liposomes are tiny spherical vesicle made by phospholipid bilayer which contained hydrophilic core and entrapped the drug to facilitated cell uptake and prevent to drug degradation. Nanostructured lipid carriers the mix of solid and liquid lipids which created imperfect matrix. In which solid lipid and drug entrapped in core and covered with liquid lipid and surfactant easily across the cell membrane.

Keywords: poor permeabilty, BCS class III, Ion-pair complex, SNEDDS, Nano-carrier

Advancing Molecular Diagnostics and Personalized Chemotherapeutic Strategies in Neuro-Oncology

Soumyadip Patra*, Arpita Biswas
[2]Department of Pharmaceutical Technology, Brainware University, Barasat-700125, West Bengal, India
10soumyadippatra@gmail.com

ABSTRACT

Brain tumours are a widespread serious neurological phenomenon that can be life-threatening, which is effectively managed by the most versatile and abruptly developing field known as Artificial Intelligence (AI) by mimicking the neural network of the human brain. This technology has act as a great support system for the researchers by capturing hidden, high-dimensional images of brain tumours. These images provide new insights into the nature of brain tumours and help to improve treatment options.AI and precision medicine (PM) are converging to revolutionize healthcare. AI has the potential to improve cancer imaging interpretation in several ways, including more accurate tumour genotyping, more precise delineation of tumour volume, and better prediction of clinical outcomes. AI-assisted brain surgery can be an effective and safe option for treating brain tumours. Various diagnostic tools including CT scan, MRI, DWI, DTI, fMRI etc. can useful methods for treatment of neuro oncology. This review discusses various AI and PM techniques that can be used in brain tumour treatment. These new techniques for the treatment of brain tumours, i.e., genomic profiling, microRNA panels, quantitative imaging, and radiomics, hold great promise for the future advancement. However, several challenges need to be addressed to facilitate these technologies to improve healthcare management.AI demonstrates substantial potential in enhancing diagnosis, prognostic assessment, and treatment planning by accurately detecting. In therapeutic management, AI contributes significantly to personalized treatment planning, protocol therapeutic planning and outcome forecasting, thereby facilitating individualized therapeutic guidance and continuous monitoring of disease progression.

Keywords: Precision medicine, brain tumours; artificial intelligence; imaging technology; gene targeting; patient care.

Computer-Aided Drug Tools for Innovation in Pharmaceutical Sciences Integrating Artificial Intelligence, Machine Learning and Computational Drug Design

Vanshika Bansal
Department of Pharmaceutical Sciences, Lovely Professional University, Phagwara, Punjab, India
bansalvanshika852@gmail.com

ABSTRACT

Procedure of recognizing drugs is expensive, time consuming and has high attrition rates. The face of pharmaceutical research is being altered by modern advancement in computer-aided drug design (CADD), artificial intelligence (AI), machine learning (ML), molecular docking, virtual screening, molecular dynamics (MD), quantitative structure–activity relationship (QSAR) modeling and generative AI making it more foretelling and data-driven. Here we look over the contemporary research literature to assess the applications of computational drug discovery tools for target recognition, structure forcasting, hit identification, lead optimization, drug redesigning, de novo molecular design and ADMET forcasting. Attention was on read up on that combined classical CADD with AI/ML and generative approaches, to assess their effect on pharmaceutical innovation. Studies reveal that computational tools can accelerate drug discovery by focusing on promising molecules and lowering inessential experimental screening. Molecular docking and virtual screening help in quick evaluation of drug–target interactions, while QSAR and ML models improve forcasting of bioactivity and pharmacokinetic properties. AlphaFold-based protein structure prediction has expanded the possibilities for structure-based drug design. protein-structure prediction has widened avenues for structure-based drug design. GenAI approaches, incorporating variational autoencoders, transformers, diffusion models and reinforcement learning, permit de novo generation and multi-faceted optimization of drug-like molecules. Incorporation of these approaches with MD and ADMET forcasting additionally refine candidate selection. However, data quality, model interpretability, generalizability, computational requirements and the requirement for experimental confirmation remain major obstacles. Computer-assisted pharmaceutical tools are powerful drivers of revolution in pharmaceutical sciences, accelerating the discovery of more effective and rational drugs. Further progress will rely on combining AI with molecular modeling, multiomics, automated experimentation and experimental pharmacology. Additional progress will rely on combining AI with molecular modelling, multi-omics, automated experimentation and experimental pharmacology.

Drug Response in the Era of Precision Medicine a Methodological Review

Ms. Apurva D Patokar
School of Pharmacy, National Forensic Sciences University Gandhinagar, Gujarat
apurvapatokar29@gmail.com

ABSTRACT

Drug response varies among patients due to molecular and phenotypic factors, highlighting the need for precision medicine to enhance treatment efficacy and minimize adverse events. Computational methods, including statistical approaches, machine learning, and deep learning, are increasingly utilized to predict individual drug responses based on large biomedical datasets. However, existing reviews often concentrate on specific diseases or techniques. Structured literature review was performed on PubMed, Scopus, and Google Scholar based on key terms pertaining to drug sensitivity/response prediction, synergy prediction, multi-omics, and statistical/machine learning/deep learning approaches, with preference to more recent articles. Title/**ABSTRACT** search for computational modeling studies followed by assessment of full text studies using a coding sheet that included the following characteristics of each study (1) type of data (structured/unstructured), (2) study design (single type of data with response vector, single type of data with response matrix, or multiple types of data with response), and (3) modeling approach (statistical, machine learning, or deep learning). Other information, including datasets used, prediction problem, integration method, validation process, and code availability, was extracted from papers and synthesized. Result Gene expression emerged as the strongest single predictor of drug sensitivity, with multi-omics integration offering only modest additional improvement. Graph neural networks performed best on relational data (e.g., protein interactions, drug structures), while convolutional networks suited imaging and grid-structured omics data. Common limitations across studies included drug identity bias from random data splits, inconsistent evaluation metrics, limited external validation, poor interpretability of DL "black-box" models, and underrepresentation of diverse patient populations. Statistical, ML, and DL approaches have had notable success in the development of accurate models of drug response prediction based on multi-omics and clinical data, although there are several barriers that prevent their implementation as reliable clinical tools, such as the lack of transparency, poor generalizability to other populations/datasets, and insufficient validation approaches. The authors recommend employing standardized and suitable validation procedures (e.g., drug or cell line leave-one-out or nested cross-validation) and improving phenotyping consistency between preclinical and clinical datasets, increasing the diversity and representativeness of data, and fostering interdisciplinary collaboration of computational, clinical, and pharmacological scientists

Keywords: Drug response prediction; Precision medicine; Machine learning; multi-omics Integration.

Artificial Intelligence-Enabled Nanotechnology for Precision Drug Delivery Current Advances and Future Perspectives

Shiksha Tripathi, Anju Singhal, Khushi Dave
School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat, India
shikshatripathi234@gmail.com

ABSTRACT

The combination of nanotechnology and artificial intelligence (AI) appears to be an effective solution in order to tackle the major problems of drug delivery, which include poor bioavailability, non-selectivity in distribution, toxicity and lack of consistency in treatment effects. The nanocarriers (liposomes, polymeric nanoparticles and dendrimers) provide controlled and targeted delivery whereas AI allows the rational design and optimization of these drug delivery systems in the framework of precision medicine. A literature review has been performed to analysed AI application in designing, optimizing and assessing of nanotechnology-based drug delivery systems. Various machine learning methods (neural networks, support vector machines, and genetic algorithms) have been analysed for their ability to predict optimal formulation and manufacturing parameters. AI-based molecular modelling and simulation of the dynamics of drug-nanocarrier interaction, cell uptake and biodistribution have been studied. Predictive power of various deep learning methods for stability, drug loading and drug release from nanocarriers has been analysed along with the possibility to consider patient-specific parameters (genomics, biomarkers, pharmacokinetics).The analysis of literature reveals that AI-assisted nanotechnology provides an improvement in design, saves time in experiments and allows to better predict formulation characteristics, release profile and targeted delivery of drugs to certain areas.AI-integrated nanotechnology appears to be a promising technique for intelligent drug delivery. Nevertheless, there still appear to be some difficulties, which require more research, and these include availability of data, reproducibility, biological complexity and translational issues. Further studies should pay attention to the development of AI-driven nanomedicine in combination with immunotherapy and biosensors.

Keywords: Artificial Intelligence; Nanotechnology; Precision Drug Delivery; Nanoparticles; Machine Learning; Targeted Therapy; Personalized Medicine; Intelligent Drug Delivery Systems

Development and Evaluation of a Palatable Quercetin Mouth-Dissolving Film Using a Sweet-Sour Taste-Masking System

Palak Kansal, Dr. Smirti Sahu
B. Pharm, KIET Deemed to Be University, Muradnagar, Uttar Pradesh, India
Palakk1386@gmail.com

ABSTRACT

Quercetin is an anti-oxidant natural flavonoid compound, which displays remarkable anti-inflammatory properties. Unfortunately, this flavonoid is less in water solubility and gives bad after taste, limiting its acceptability for oral use. Thus a mouth dissolving film can serve as convenient oral dosage form rapidly disintegrates in oral cavity and can improve patient compliance. The objective of this study is to develop a palatable mouth dissolving film of quercetin by utilizing a sweet-sour taste masking technique. Mouth dissolving films of Quercetin were prepared by solvent casting method using a appropriate film forming polymer and plasticizer. A sweet and sour taste-masking system was to consist of sweetening agents, fruit flavor and citric acid were formulated with the selected taste buds. Formulations with variation concentration of taste-masking ingredient would be released. Physicochemical characteristics namely physical appearance, thickness, weight variation, folding endurance, surface pH, drug content, disintegraton and in-vitro drug released should be evaluated and analyzed. Optimised formulation will be selected and characterised on based of physicochemical and release profiles. The film prepared are expected to be having uniform appearance, flexibility, good drug contents, fast disintegration rate and most importantly appealing taste. The optimized formulation will be selected based on the comparative evaluation of the prepared formulations. The study is proposed to develop and screen a palatable mouth dissolving film for Quercetin utilizing the principle of the sweet and sour systems and to investigate their therapeutic efficacy to improve the suitability of orally administrated Quercetin.

Keywords: Quercetin, Mouth-dissolving film, Taste masking, Sweet-sour system, Oral film, Solvent casting.

Beyond One-Size-Fits-All MHT Pharmacological and Pharmacogenomic Approaches to Personalized Menopausal Care.

Bhumika Bohra*, Jainee Vashi
Department Of Pharmacology, Parul Institute of Pharmacy And Research, Parul University, Vadodara, Gujarat, India
bhumikabohra26@gmail.com

ABSTRACT

Menopause brings flashes, bladder problems, trouble sleeping, mood swings and bone loss. Menopausal hormone therapy or MHT is still the drug to stop hot flashes and keep bones healthy. How well MHT works and how safe MHT is can differ a lot from one woman to another. A personalized plan that looks at both medicines and genes might make MHT treatment better. This review wants to show medicines and gene tests that can tailor care and to see how they might improve how well MHT works while keeping MHT safe. We looked at studies about estrogen and progestogen drugs how they are given, the right dose and how genes that affect estrogen receptors and metabolism might change the response. The evidence shows that choosing the type of hormone the right dose, how it is given and how long it lasts should be based on a woman's age how long it has been since menopause how bad the symptoms are, health problems and a woman's personal risk. Using estrogen patches and lower doses can lower the chance of blood clots and stroke in some women. Gene studies point to differences in ESR1, ESR2 and SULT1A1 that might explain why hormone response varies. But the are mixed and gene testing is not yet ready for MHT choice. Menopause care should go beyond a plan, for everyone. Menopause care should combine a woman's risk profile, MHT choices and maybe gene markers. We need studies to prove that using a woman's genes can guide MHT and to create clear useful rules that make menopausal care safer and better.

Keywords: Menopausal hormone therapy, Menopause, Estrogen patches, ESR1, ESR2, SULT1A1, Woman's risk profile.

Precision Cardiology in Patients with Thyroid Disorders Integrating Molecular Biomarkers, Polypharmacy and Personalized Cardiovascular Risk Assessment

Nupur Nitin Barbare*, Zalak Shah
Department Of Pharmacology, Parul Institute of Pharmacy And Research, Parul University, Vadodara, Gujarat, India
nupurbarbare@gmail.com

ABSTRACT

Thyroid disorders are a deal when it comes to heart problems. They can really affect how your heart works. This is because thyroid disorders change things like the fat in your blood how hard your blood vessels work, your heart rate and how well your heart squeezes. Usually when doctors check your risk of heart problems they do not think about how your thyroid's working. This is why we need to be more precise when we are trying to figure out your risk. We want to see if looking at signs in your blood and all the medicines you are taking can help us understand your risk of heart problems better if you have a thyroid disorder. We looked at what other researchers have found out about how thyroid problems connected to heart disease. We talked about tiny signs in your blood like thyroid-stimulating hormone, free triiodothyronine, free thyroxine and some other markers that can tell us about your heart health. We also thought about how taking a lot of medicines can affect your heart and what happens when these medicines interact with each other. What we found out is that if we look at your thyroid and heart health at the time we can find people who are at high risk of heart problems earlier. If we look closely at all the medicines you are taking, we might be able to stop interactions between them make sure your medicines are working well and understand your risk of heart problems better if you have a thyroid disorder. Precision cardiology is a way to take care of your heart that's just right for you especially if you have a thyroid disorder. It involves looking at signs in your blood and all your medicines. This way of taking care of your heart might help us predict who is, at risk make sure you are taking the medicines and help doctors make good decisions about your care. We need to do research to see if this works in everyday doctor visits.

Keywords: Thyroid disorders, Heart disease, Thyroid-stimulating hormone, Free triiodothyronine, Free thyroxine, Precision cardiology.

Mucoadhesive Nanogels for Nose-to-Brain Delivery of Anti-Migraine Drugs Bridging Nanotechnology and Clinical Translation

Sparsh Verma[1], Dr Snigdha Bhardwaj[2]
Department of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
sparshv24@gmail.com

ABSTRACT

Migraine remains one of the most disabling neurological conditions worldwide, yet standard therapies work against the disease itself. Oral drugs depend on gut absorption that nausea and vomiting routinely disrupt, while injections avoid this but bring invasiveness and poor acceptance. Both are further limited by the blood-brain barrier, which restricts CNS penetration of many otherwise effective molecules. The nasal route offers a way around much of this drug applied to the nasal cavity can reach the brain along olfactory and trigeminal pathways, bypassing hepatic first-pass metabolism. Mucoadhesive nanogels are gaining attention here, since their ability to adhere to nasal mucosa extends residence time well beyond what a simple spray allows. This is a critical literature review, not an experimental study. Published work on intranasal nanocarriers, mucoadhesive polymers, nanogel formulations, anti-migraine drugs, and nose-to-brain transport mechanisms was examined and synthesized, with particular attention to translational barriers. Reviewed evidence shows intranasal nanocarriers can prolong nasal residence, enhance mucosal permeation, protect labile drugs from degradation, and enable more direct CNS access. One recurring issue deserves attention many reported "nanogels" are actually nanoparticle-loaded gels or in-situ gelling systems rather than true polymeric nanogels a distinction this review draws deliberately. Persistent gaps include sparse clinical data, uncertain long-term nasal safety, inconsistent large-scale manufacturing, unresolved stability and device-compatibility questions, and an unclear regulatory pathway. Mucoadhesive nanogels represent a promising but still largely unproven platform for CNS-targeted anti-migraine delivery. Progress will require rational formulation design, rigorous safety evaluation, scalable manufacturing, and well-designed human studies.

Keywords: mucoadhesive nanogel; nose-to-brain delivery; intranasal drug delivery; anti-migraine drugs; blood–brain barrier; nasal mucosa; clinical translation

Digital Nanomedicine Integrating Artificial Intelligence andComputer-Aided Design for Next-Generation Drug Delivery Systems

Debasis Sethi*, Dr. Nihar Ranjan Kar 1
1 Department of Pharmaceutics, School of Pharmacy and Life Sciences,
Centurion University of Technology and Management, Balasore-756044, Odisha, India
debasissethi04@gmail.com

ABSTRACT

Nanotechnology has emerged as a versatile platform for improving drug delivery by enhancing solubility, stability, bioavailability, cellular uptake, and controlled release. However, designing an optimized nanocarrier involves complex interactions among formulation components and process variables. Digital nanomedicine, integrating artificial intelligence (AI) and computer-aided design (CAD), offers a rational approach to address these challenges. Relevant scientific literature on AI, machine learning, computer-aided formulation design, nanocarriers, and Quality by Design (QbD) was examined to understand their applications in pharmaceutical nanotechnology. The role of computational models in predicting critical quality attributes, optimizing formulation variables, selecting excipients, and establishing predictive design spaces was evaluated. AI and machine learning can identify relationships between formulation variables and critical quality attributes such as particle size, polydispersity index, zeta potential, encapsulation efficiency, and drug-release behaviour. Computer-aided modelling can support the selection of polymers, lipids, surfactants, and other excipients by assessing drug–excipient interactions and formulation compatibility. Integration of these approaches with QbD can reduce repetitive experimental trials, improve formulation optimization, and support the development of more robust nanocarriers. These computational strategies can also facilitate early-stage screening and reduce unnecessary formulation iterations during nanocarrier development. However, dataset quality, model interpretability, reproducibility, and experimental validation remain important challenges. The integration of AI, CAD, and nanotechnology represents an emerging digital framework for more predictive and efficient drug delivery development. Properly validated computational approaches may reduce development time and experimental burden while supporting the design of precise, reproducible, and patient-oriented nanocarrier systems.

Keywords: Digital nanomedicine; Artificial intelligence; Machine learning; Computer-aideddesign; Nanocarriers; Quality by Design; Drug delivery.

Artificial Intelligence for Toxicology and ADMET Assessment Accelerating Safety Testing in Medication Development

Manish Joshi
School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat, India
manish.joshi0057@gmail.com

ABSTRACT

The field of pharmaceutical development still experiences difficulties owing to the high attrition rates experienced during the late stages of drug development, with majority of these problems resulting from unfavourable pharmacokinetics and clinical toxicity. The ADMET process is not only expensive but also time consuming and resource demanding both in the in vitro and in vivo conditions. At the first hit-to-lead selection process, the combination of artificial intelligence (AI) and machine learning (ML) algorithms provides a computational paradigm for predicting drug liability and drug likeness. The standard databases for molecular properties and benchmark data sets for bioactivities (ChEMBL, Tox21) have been used for an organized in silico study. The performance of machine learning models namely Random Forest (RF), Support Vector Machines (SVM), and Graph Neural Networks (GNN) was evaluated along with the popular computational tools available in public domain, like SwissADME, pkCSM, and ProTox-II. The ADMET features investigated using the descriptors of two-dimensional and three-dimensional molecules include gastrointestinal absorption, blood-brain barrier permeation, cytochrome P450 isoforms inhibition, hERG-induced cardiotoxicity, and Ames mutagenicity. Classification accuracy for cross-validation was found between 78% and 91%, ROC-AUC was more than 0.84 for vital safety endpoints, indicating that highly advanced machine learning techniques exhibited excellent prediction power in various areas of chemical sciences. For efficient screening of chemical compounds prior to synthesis in laboratory and to ensure that certain toxic alerts are not missed by the system, deep learning as well as graph-based models performed better. In rational drug design, the use of artificial intelligence for ADMET screening serves as a very effective initial filter to decrease the experimental synthesis burden and comply with 3Rs regulation. Initial computational toxicology plays an important role in minimizing risks of development strategies even though in vitro validation remains necessary.

Keywords: Artificial Intelligence; ADMET Profiling; Computational Toxicology; Machine Learning; QSAR; Drug Safety Screening.

Artificial Intelligence in Pharmaceutical Regulatory Governance Opportunities, Challenges, and Future Directions for the Indian Pharmaceutical Industry

Krishna Mohapatra[1], Pawan Pandey[1]*
[1]Department of Pharmaceutics, College of Pharmacy, JSS University, Noida-201301, Uttar Pradesh
mohapatrakrishna56@gmail.com

ABSTRACT

Pharmaceutical regulatory concerns are being revolutionised by artificial intelligence (AI), which increases productivity, precision, and adherence across the product lifecycle. Regulatory agencies like the European Medicines Agency and the U.S. Food and Drug Administration are increasingly relying on sophisticated data systems, which opens the door to AI-driven applications in lifecycle management, pharmacovigilance, dossier preparation, and regulatory intelligence, audit automation, document validation, minimizing risks associated with non-compliance and regulatory reporting. Automated document reviews, data validation, signal detection, and predictive regulatory strategy are supported by technologies like machine learning and natural language processing. There are still issues with data integrity, transparency, validation, and regulatory approval in spite its benefits. India has ingrained culture of paper centric quality assurance which creates a major gap such as vulnerability to errors and frauds, insufficiency and resource misallocation, the integration of Robotic Process Automation (RPA) and low-code AI to automate pharmaceutical compliance workflows, addressing regulatory inefficiencies This analysis focuses on the main uses, advantages, and potential future developments of artificial intelligence in pharmaceutical regulatory concerns. This review further focuses on the use of AI and machine learning in Indian pharmaceutical companies to address challenges related to data integrity, ensuring the reliability and traceability of information. The review emphasizes the scalability of AI-driven solutions in handling vast datasets and extracting valuable insights, thereby facilitating proactive regulatory strategies and exploring the future role of artificial intelligence in pharmaceutical regulatory governance.

Keywords: Artificial Intelligence (AI), Natural Language Processing (NLP), Machine Learning (ML), Robotic Process Automation (RPA), Clinical Trials, Electronic Health Records (EHR), Data Privacy.

Decoding the Microbial–Epigenetic Connection in Silico Target Discovery of Fresh Fruit-Associated Bacterial Metabolites

Prayukta Padelkar[a], Ashutosh Tripathi [b], Anuradha Jayaraman [c], Rinkal Patel [d], Sanjeevi Ramakrishnan [c*]
a Department of Genetics, Nims Institute of Allied Medical Science and Technology, Nims University Rajasthan, Jaipur - 303121.
b Nims Institute of Engineering and Technology, Nims University Rajasthan, Jaipur - 303121.
c Nims Institute of Allied Medical Science and Technology, Nims University Rajasthan, Jaipur - 303121.
d Director, Rapture Biotech, Mumbai, Maharashtra, India - 400064.
r.sanjeevi@nimsuniversity.org

ABSTRACT

Fruit-associated microbes represent an unexplored repository of physiologically active metabolites that may affect host–microbe relationships beyond the gastrointestinal tract. Specifically, gut bacterial function, host signalling, and the gut–brain axis could potentially be linked at the molecular level via bacterial metabolites. However, the host-specific targets and mechanisms governing such interactions remain poorly characterized. Therefore, this study explores the potential of fruit-associated bacterial metabolites as molecular mediators of host biological processes, with particular emphasis on pathways relevant to the gut–brain epigenetic interface. Microbiological, molecular, and phylogenetic methods were employed to characterize bacteria associated with asymptomatic and symptomatic fruits. Selected microbial isolates were subjected to metabolite profiling using NMR spectroscopy. N-acetyl-L aspartic acid and 4-hydroxyphenylacetic acid were among the recurrent metabolites detected across multiple bacterial isolates and were prioritized for CADD-based investigation. The computational workflow enabled assessment of their physicochemical properties, predicted human molecular targets, and metabolite–target interaction profiles. Target and pathway mapping provided potential associations with neurotransmission, host signalling, and epigenetic regulatory processes. The integration of microbial characterization, NMR-based metabolite profiling, and CADD-driven in silico analysis provides an experimental-to-computational framework for examining the microbial metabolite gut–brain epigenetic interface and generating testable mechanistic hypotheses for further experimental verification.

Keywords: Fruit-associated bacteria, Microbial metabolites, NMR metabolomics, Computer-aided drug design, In silico target prediction, Gut–brain axis, Host–microbe interactions, Epigenetic regulation.

Artificial Intelligence in Drug Discovery and Development During COVID-19 and Vaccine Formation

Anusree Golui[1*], Anisur Rahaman Molla [1]

Maharishi School of Pharmaceuticals, Maharishi University of Information Technology, Noida, Uttar Pradesh, 201304

goluianusree@gmail.com

ABSTRACT

The COVID-19 pandemic revealed critical limitations in traditional drug discovery and vaccine development approaches, which are often slow and resource-intensive. Artificial intelligence (AI) emerged as a transformative technology, accelerating therapeutic identification and vaccine design.This review aims to evaluate the role of AI in drug discovery and vaccine development during the COVID-19 pandemic, emphasizing its applications, outcomes, and limitations.A comprehensive literature review was conducted on peer-reviewed articles, reports, and clinical trial data published between 2020 and 2025, focusing on AI-driven platforms, machine learning algorithms, and computational models applied to SARS-CoV-2 research.AI enabled rapid virtual screening of large compound libraries, identification of repurposed drugs such as remdesivir and baricitinib, and prediction of novel antiviral candidates. Structural modeling of the SARS-CoV-2 spike protein supported the design of mRNA vaccines by Moderna and Pfizer-BioNTech. In addition, AI optimized clinical trial design, patient stratification, and post-market safety monitoring, significantly reducing development timelines and enhancing translational outcomes.AI demonstrated transformative potential during the COVID-19 pandemic by bridging computational science with pharmaceutical innovation. Despite these advances, challenges remain in data standardization, algorithm transparency, ethical considerations, and regulatory acceptance. Addressing these barriers is essential to establish AI as a reliable and integral component of future pandemic preparedness and routine drug development pipelines.

Keywords: Artificial Intelligence, COVID-19, Drug Discovery, Vaccine Development, Machine Learning, mRNA Vaccines

Global and India- Specific Insights into Cervical Cancer Epidemiology, Prevention, Diagnostics, and Therapeutic Advances

Jeet Nabam
[1]* School of Pharmaceutical Sciences, Maharishi University of Information Technology, Noida, Uttar Pradesh, 201304
nabamjeet13@gmail.com

ABSTRACT

Cervical cancer is the fourth most common cancer and cause of cancer-related death among women globally, with 660,000 new cases and 350,000 deaths in 2022. Nearly 90% of cases occur in low- and middle-income countries due to limited access to human papillomavirus (HPV) vaccination, screening, and treatment. Persistent infection with high-risk HPV types, particularly 16 and 18, is the primary etiological factor. In India, cervical cancer ranks second among cancers affecting women, with a burden of 223.8 DALYs per 100,000 in 2016 and projections of 1.5 million DALYs nationally by 2025, with higher incidence in northeastern states. This **abstract** synthesizes global and India-specific epidemiological data, prevention strategies, diagnostic advances, and treatment approaches for cervical cancer. Key sources include registry data, WHO reports, and recent diagnostic imaging studies. High-income countries have reduced incidence and mortality by over 50% in the past three decades through widespread Pap smear screening and HPV vaccination. Diagnostic innovations, such as multisequence MRI with radiomics–deep learning integration, have achieved high predictive accuracy (AUC ≈ 0.90) for occult lymph node metastasis. Early-stage disease is often managed surgically, while stages IIB–IVA are treated with concurrent chemoradiotherapy, with intensity-modulated radiotherapy reducing toxicity. Bevacizumab has improved median survival beyond 12 months for recurrent/metastatic cases, and emerging immunotherapies show promise. Reducing the global cervical cancer burden requires scaling up HPV vaccination, implementing cost-effective screening, integrating advanced diagnostics, and ensuring equitable access to modern therapies, especially in resource-constrained regions.

Keywords: Cervical Cancer, Human papillomavirus, Screening, Diagnostic imaging, Chemoradiotherapy,

An AQbD-Driven Green Stability-Indicating UFLC Method for Quantification of SecoisolariciresinolDiglucoside from Linum usitatissimum and Its Relevance in PCOS

Anusha N, Souhardya Santra, Karthika Paul
Department of Pharmaceutical Chemistry, JSS College of Pharmacy, JSS Academy of Higher Education and Research, Mysuru, Karnataka, India
souhardyasa2003@gmail.com

ABSTRACT

Polycystic ovary syndrome (PCOS) is a complicated metabolic and endocrine disorder characterized by insulin resistance, oxidative stress, and hormonal imbalance. In addition, dysfunctions in regulatory pathways such as AMPK and SIRT1 are major contributors to its pathogenesis. Secoisolariciresinoldiglucoside (SDG), a type of lignan derived from flaxseed (Linum usitatissimum), shows how good its body's ability is to generate energy, metabolism, and resistance to damage from free radicals. However, the ability to accurately study SDG has been limited because sustainable extraction techniques and reliable green analytical methods do not yet exist. The goal of this study was to develop a green extraction method for SDG, create an AQbD-based RP-UFLC method to measure SDG, and to evaluate its potential uses through making in silico measurements. SDG was extracted using a surfactant-assisted microwave assisted green extraction method and characterized through TLC, FT-IR and ^{1}H NMR. The chromatography for SDG was then done using Shimadzu UFLC system with PDA detection and BDS Hypersil C18 column (200 × 4.6 mm, 5 µm). Mobile phase composition was ethanol water at a ratio of 2080 (v/v) with the addition of 0.1% glacial acetic acid and flow rate of 1 mL/min was used for method optimization and validation according to ICH guidelines. The method produced a retention time of approx. 4.08 minutes; with high linearity, R^2 0.9999, y = 8130.7x−8219.6, and 98–102% accuracy with %RSD less than 2%, for precision; LOD and LOQ were 0.33 µg/mL and 1.00 µg/mL respectively; the forced degradation studies confirmed the stability-indicating nature of this method; the in silico analysis showed strong binding affinities, stable interactiveness, and good safety profiles of SGD vs. Resveratrol. The method is robust, sensitive, and environmentally sound and shows SGD is a good candidate to help with PCOS.

Keywords: SDG, PCOS, RP-UFLC, AQbD, Green Extraction, Molecular Docking

Microfluidic Device for Adulteration Detection In Food And Milk A Rapid, Sensitive And Cost-Effective Analytical Approach

Babaloo Kumar Yadav *Ms. Pallavi Barik
* Department of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
babaloo.2327bph1074@kiet.edu

ABSTRACT

Food and milk adulteration is a major public health concern that can compromise food quality and consumer safety. Conventional methods for adulteration detection may require skilled personnel, expensive instruments, and considerable analysis time. Microfluidic technology offers a rapid, sensitive, portable, and cost-effective approach by enabling sample handling and chemical reactions within miniaturized microchannels. The present study focuses on the development of a microfluidic device for the rapid detection of common adulterants in milk and food samples using small sample and reagent volumes. A microfluidic device was designed using polydimethylsiloxane (PDMS) with micrometer-scale channels fabricated by soft lithography. The device consists of sample and reagent inlets, a micromixing channel, and an outlet detection zone. Samples were collected and prepared before loading into the microfluidic device, followed by micromixing with specific reagents. Urea in milk was detected using diacetyl monoxime and thiosemicarbazide, starch using iodine solution, detergent using methylene blue, and argemone oil in edible oil using p-anisidine reagent. Sudan Red IV in food was addressed through solvent extraction followed by microfluidic detection. The detection response was assessed by visible color change, with possible readout by naked eye, smartphone, or spectrophotometer. Argemone oil in edible oil produced yellowish-green, green, and dark-green responses at concentrations of 1%, 2%, and 5%, respectively, with a detection time of approximately 4 minutes. These findings demonstrate the potential of the device for rapid screening using low sample and reagent consumption. The developed microfluidic device provides a simple, rapid, sensitive, portable, and cost-effective approach for detecting common adulterants in milk and food samples. Its miniaturized design reduces sample and reagent consumption while providing clear visual within a few minutes. The device has potential applications in milk quality monitoring, edible oil purity testing, food safety and quality control, on-site testing, and public health protection.

Keywords: Microfluidic device; Food adulteration; Milk adulteration; Urea; Starch; Detergent; Argemone oil; Colorimetric detection; Food safety.

Phytoconstituent-Mediated Drug Delivery for Gastritis A Review on Synergistic Mechanisms and Therapeutic Potential"

Pushpika Jain[1], Dr. Yogendra Singh[2]
Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
MVN University, Palwal, Haryana
pushpikajain25@gmail.com

ABSTRACT

Gastritis is still major gastrointestinal condition in the world, and they are frequently linked to Helicobacter pylori infection, inflammation, oxidative stress, and excessive gastric acid production. Despite its effectiveness, conventional pharmacotherapy which includes proton pump inhibitors and H_2-receptor antagonists is frequently constrained by medication resistance, side effects, and low patient compliance. The medicinal potential of phytoconstituents with antioxidant, anti-inflammatory, antibacterial, and mucosal protecting qualities, such as flavonoids, alkaloids, saponins, and terpenoids, has been brought to light by recent studies. Phytoconstituents provide a synergistic therapeutic strategy by reducing adverse effects and increasing pharmacological efficacy when combined with traditional medications. Furthermore, the bioavailability and targeted release of these bioactive chemicals have been enhanced by sophisticated drug delivery technologies, such as polymeric carriers, in situ gels, and nanoparticles, promising superior clinical. This study discusses the mechanisms of action, delivery methods, and potential future research areas of drug-loaded phytoconstituents, offering a thorough overview of their synergistic function in the treatment of gastritis and peptic ulcers. One approach that shows promise for creating safer and more efficient gastroprotective treatments is the combination of contemporary pharmaceutics and natural therapies.

Keywords: Gastritis, Phytoconstituents, Synergistic Therapy, Insitu Gels, Mucoadhesive Release

In-Silico Design of Nano-Phytoconstituent Based Topical Gel for Anti-Arthritic Activity a Computational Approach

Vikhyat
Department of Pharmacognosy, VIIT Pharmacy College, Bulandshahr, Uttar Pradesh, India
rajvikhyat13@gmail.com

ABSTRACT

Arthritis is *a* chronic inflammatory disorder affecting joints, driven by cyclooxygenase-2 (COX-2) mediated inflammation. Curcumin from *Curcuma longa* shows potent anti-inflammatory activity via selective COX-2 inhibition but suffers from poor solubility and low systemic bioavailability. The chemical structure of curcumin (CID 969516) and the crystal structure of COX-2 (PDB ID 5KIR) were retrieved from online repositories. Molecular docking was performed via CB-Dock2 / AutoDock Vina to determine binding affinities. ADMET profiles were predicted using SwissADME and pkCSM online tools. A topical delivery system was designed formulated as a chitosan-based polymeric nanogel. Molecular docking revealed a strong binding energy of -8.2 kcal/mol, showing key interactions with residues Arg120, Tyr385, and Ser530 of the COX-2 active site. ADMET predictions indicated high gastrointestinal (GI) absorption, zero Lipinski rule violations, no hepatotoxicity, and a low risk for skin sensitization. The optimized nano-gel matrix exhibited a theoretical size of ~120 nm with a Poly-dispersity Index (PDI) <0.2. The *in-silico* data suggests that the curcumin-loaded nano-gel is a promising, safe, and highly permeable candidate for topical anti-arthritic therapy, warranting further *in-vitro* and *in-vivo* experimental validation.

Keywords: Curcumin, COX-2, Molecular Docking, SwissADME, Nano Gel, Anti-Arthritic.

Polypharmacology – A Multi-Target Approach to Drug Discovery

Ishita B. Vekariya*1, Bina Maradia2
1M. Pharm, Final Year Student, Faculty of Pharmacy, Dr. Subhash University, Junagadh
2Assistant Professor, School of Pharmacy, Dr. Subhash University, Junagadh
ishitavekariya58@gmail.com

ABSTRACT

Polypharmacology is an emerging concept in modern drug discovery that refers to the ability of a single drug to interact with multiple biological targets. Unlike the traditional "one drug-one target" approach, polypharmacology considers the complex nature of diseases involving multiple interconnected pathways. Multi-target interactions may improve therapeutic efficacy and provide synergistic effects, particularly in complex diseases such as cancer, neurological disorders, cardiovascular diseases, and infectious diseases. Advances in network pharmacology, molecular docking, systems biology, and artificial intelligence have facilitated the identification and prediction of drug-target interactions. However, unintended target interactions can also produce adverse effects and toxicity. Therefore, understanding polypharmacological profiles is essential for developing effective and safer therapeutic agents. Polypharmacology represents an important shift toward a network-based understanding of drug action and offers promising opportunities for developing more effective therapies for complex diseases. Integrating computational approaches with experimental validation and clinical research may enable the rational design of safer and more selective multi-target drugs. Thus, polypharmacology has significant potential to contribute to the development of next-generation therapeutics.

Keywords: Polypharmacology, Modern drug discovery, multi-target drugs, Therapeutic efficacy, Multi–target interactions, Synergistic effects.

Magnetic Nanotheranostics for Herbal Anticancer Phytochemicals Overcoming Bioavailability Barriers Through Targeted, Stimuli-Responsive Delivery

Sachin Rajawat, Meenakshi B.
Patel School of Pharmacy, Parul University, Vadodara, Gujarat, India - 391760
2508422110009@paruluniversity.ac.in

ABSTRACT

Phytochemicals with anti-cancer properties, such as curcumin, withaferin A, berberine, quercetin, resveratrol, EGCG, thymoquinone, and genistein, interfere with cancer-inducing pathways (PI3K/Akt/mTOR, NF-κB, MAPK, Wnt/β-catenin, and STAT3) and induce apoptosis with relatively mild systemic toxicities. However, their further clinical translation is hindered due to low water solubility, poor bioavailability via an oral route, fast metabolism, and lack of selective biodistribution. The magnetic nanotheranostic platforms that are developed based on superparamagnetic iron oxide nanoparticles (SPIONs) and functionalized with PEG, chitosan, dextran, hyaluronic acid, and PLGA overcome these obstacles by increasing the stability of encapsulated phytochemicals, providing for a prolonged time of circulation, and delivering the drugs via external magnetic guidance to tumors. Additionally, these systems can combine drug release in response to stimuli, hyperthermia by application of a magnetic field, and T2-weighted MRI contrast in one platform and provide opportunities for concurrent diagnosis and treatment. In this paper, formulation approaches, surface modification methods, and targeting strategies of herbal magnetic nanotheranostics that have been proposed during 2020-2026 years will be reviewed. Special attention will be paid to the performance of magnetic nanoparticles in terms of protein corona formation, endosome escape, and tumor accumulation. Emerging trends such as AI/ML-assisted formulation development, quality-by-design (QbD) paradigm, and co-loading of multifunctional nanoparticles are discussed as facilitators for clinical translation. Nevertheless, herbal variability, scale-up of production under cGMP conditions, toxicity from iron accumulation, and the lack of unified nano-specific guidelines hinder further advancement of this field.

Keywords: Superparamagnetic iron oxide nanoparticles (SPIONs); Herbal phytochemicals; Nanotheranostics; Targeted drug delivery; Stimuli-responsive release; Bioavailability enhancement; Magnetic resonance imaging (MRI)

Mesoporous carbon-containing voltammetric biosensor for determination of tyramine in food products

Akansha Sharma, Ms Pallavi Barik*
Department of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
akansha.2428bph2699@kiet.edu

ABSTRACT

The developed tyrosinase-based voltammetric biosensor provides a sensitive and reliable approach for tyramine detection. Its good analytical performance and applicability to food samples indicate its potential for rapid monitoring of tyramine levels and assessment of food quality and safety. The combination of tyrosinase with conductive carbon materials and the supporting polymer matrix enhances the electrochemical response and provides an effective platform for detection. Therefore, this biosensor can be considered a promising analytical tool for food analysis and quality-control applications. A voltammetric biosensor based on tyrosinase (TYR) was developed for the determination of tyramine, a biogenic amine commonly present in fermented and processed food products. Carbon materials, including multi-walled carbon nanotubes or mesoporous carbon CMK-3-type, along with the polycationic polymer poly(diallyl dimethylammonium chloride) (PDDA) investigated using scanning electron microscopy (SEM) and cyclic voltammetry (CV). The and Nafion, were incorporated into a titanium dioxide sol (TiO_2) to form an immobilization matrix. The structural and electrochemical characteristics of the developed matrix where analytical performance of the biosensor was evaluated in terms of linear range, sensitivity, limit of detection, long-term stability, repeatability, and reproducibility. The developed biosensor exhibited electrocatalytic activity toward tyramine oxidation and showed a linear response over the concentration range of 6–130 µM. It demonstrated high sensitivity of 486 µA mM^{-1} cm^{-2} and a limit of detection of 1.5 µM. The apparent Michaelis–Menten constant was calculated to be 66.0 µM, indicating good biological affinity of the immobilized tyrosinase toward tyramine. The biosensor also showed satisfactory analytical performance and was successfully applied to the determination of tyramine in food product samples. The developed tyrosinase-based voltammetric biosensor demonstrated effective and reliable detection of tyramine in food products. The incorporation of conductive carbon materials and the supporting polymer matrix enhanced the electrochemical response and provided good sensitivity, stability, and reproducibility. Its successful application to real food samples highlights its potential as a rapid and convenient analytical tool for monitoring tyramine levels. Therefore, this biosensor can be considered a promising approach for food quality assessment, safety monitoring, and quality-control applications.

Keywords: Biosensor; Tyrosinase; Tyramine; Voltammetric detection; Food analysis; Food safety.

Determination of cadmium in different groundwater samples by complexometric principle and atomic absorption spectroscopy A comparative study

Akshita Sharma, Ms. Pallavi Barik*
Department of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
akshita.2428bph2749@kiet.edu

ABSTRACT

This work describes analytical approaches based on simple complexometric principle leading to the colour change of a novel microfluidic cloth-based analytical device (μCAD). The device was fabricated using the wax dipping method of cotton fabric. Then the fabric was treated with an indicator solution, providing an easy-to-use platform for rapid measurement of analyte concentration in aqueous solution. Interaction between the deposited reagents and analytes in the samples then occurred within a few minutes. This resulted in zones of colour change with different colour intensities depending on the analyte concentration. The interaction zones can be analyzed by imageJ software based on a comparison of the colour intensity with the printed scales which are correlated with the analyte concentrations. The complexometric principle using μCADs was used for the investigation of cadmium metal in standard samples along with groundwater samples in nearby region. The device was pretreated with EDTA and citric acid followed by xylenol orange indicator. A pH of 9 was maintained throughout the reactions for better colour intensity. Then load the sample on the fabric which in reddish-brown colour which is directly proportional to the concentration of Cd2+ in the water sample. The working concentrations was 20ppm-60ppm. Further, the LoD and LoQ of the device was found to be 3.84ppm and 11.60 ppm respectively. The developed method was applied in analysis with real groundwater samples which showed being in agreement with those obtained in atomic absorption spectroscopy. The developed method was applied in analysis with real groundwater samples which showed being in agreement with those obtained in atomic absorption spectroscopy.

Keywords: Cadmium; Groundwater samples; Complexometric principle; Atomic absorption spectroscopy; Microfluidic cloth-based analytical device (μCAD)

AI-Driven Formulation Design for Advanced Drug Delivery

Pooja Markande, Khushi Dave
Pharmaceutical Quality Assurance School of Pharmacy, National Forensic Sciences University, Gandhinagar, Gujarat.
poojamarkande00@gmail.com

ABSTRACT

For tackling the needs of global healthcare, medication toxicity issues, as well as the issues of supply chain disruptions, shortage of skilled workforces, and inefficient clinical trials – all these challenges that were magnified during the COVID-19 outbreak – the pharmaceutical industry is always searching for innovative approaches. Most of the aforementioned industry challenges could be overcome by employing artificial intelligence (AI), which proved to be an innovative tool that has the ability to use large amounts of biological data such as genomics and proteomics to target diseases and drugs. The areas of drug discovery, formulation design, drug delivery systems optimization, and PK/PD studies are included in this comprehensive review of the use of AI in the drug development process. Apart from an assessment of the current limitations of AI in pharmaceutical technologies, machine learning algorithms were evaluated in terms of their application to process/formulation optimization, PK/toxicity predictions, and experimental design. AI enhances the efficiency and efficacy of drug discovery, thus reducing development costs and increasing the chances of getting approval for the drugs. Optimization and prioritization of lead chemicals can be achieved using machine learning models, which greatly reduce the cost and time associated with animal trials. While AI-powered analysis of real-life patient data helps to promote personalized medicine approach, increasing effectiveness of treatment and compliance of patients, AI-based PBPK models facilitate drug distribution/clearance simulations and prediction of pharmacokinetic parameters. A radical shift is taking place in the drug delivery process due to AI, enabling the creation of personalized and adaptive drugs. The pharma industry is now transitioning from Era 4.0 to Era 5.0 because of the continuous advancements in AI-powered computational pharmaceutics that provide a better way to formulate medicines and ensure compliance.

Keywords: Pharmacokinetics, pharmacodynamics, PBPK modeling, QSAR modeling, drug discovery, formulation, dosage form evaluation, artificial intelligence (AI), and machine

Leveraging AI and Machine Learning to Strengthen Pharmacovigilance Systems

Suryansh Chauhan[1], Anuj Kr. Singh Jadon[1]
Department of Pharmaceutical Chemistry, College of Pharmacy JSS University, Noida 201301, India
suryansh.ch.jssate@gmail.com

ABSTRACT

Pharmacovigilance is an important aspect that involves recognition of risks linked with drugs. Nevertheless, many current models continue to rely on the use of spontaneous reports, manual processing, and statistical approach, which may be constrained by underreporting, biasedness and increasing amount of safety data. AI and machine learning (ML) represent modern opportunities for addressing these issues.To explore how AI and ML technologies have been employed in the area of pharmacovigilance and to discuss the advantages and disadvantages of their application.To assess their use for the identification of safety signals, detection of adverse drug reactions (ADRs) and other pharmacovigilance tasks.Narrative review of literature was conducted based on NLP, deep learning, knowledge graph and federated learning applications.The methods such as BCPNN, MGPS, MADEx, and gradient boosting had higher performance compared to conventional disproportionate analysis, with AUC ranging to 0.96. NLP techniques demonstrated F-scores of 0.97 for the detection of ADRs. The examples from FDA's Sentinel initiative and UMC's vigiMatch also indicate that the AI approaches are applicable in the real-life scenario in pharmacovigilance. Still, there is a number of challenges, including data quality, bias, model explainability, regulatory needs, and causation. The application of AI and ML could enhance the detection of ADRs earlier and more reliably. For their efficient application, it is necessary to have good data quality, model transparency, and human control.

Keywords: Pharmacovigilance; Artificial Intelligence; Machine Learning; Adverse Drug Reactions; Signal Detection

pH- and Microbiota-Responsive Multiparticulate Pellet Systems for Colon Targeted Delivery of Sulfasalazine in Ulcerative Colitis A Review

Sougata Ghosh1, Dr. Meenakshi B. Patel1*
Pharmaceutics Department ,1School of Pharmacy, Parul University, Vadodara, Gujarat, India.
meenakshi.patel24771@paruluniversity.ac.in

ABSTRACT

Ulcerative colitis (UC) is a chronic inflammatory disease of the colon, which requires targeted delivery of the drug in order to limit systemic exposure and maximize local therapeutic effect. Sulfasalazine is one of the azo-bond prodrugs that have inherent colon-targeting property and has been used conventionally for treatment of UC. But conventional sulfasalazine tablets do not utilize this property of the drug maximally. A review of literature regarding colon-targeted multiparticulate delivery system of sulfasalazine pellets was conducted. The focus was on the method of pellet preparation (extrusion spheronization or layering); choice of core and excipients of sulfasalazine; pH-dependent and microbiota activated coatings of particles made up of polymers (Eudragit L100/S100) and polysaccharides (guar gum, pectin), in vitro and in vivo studies on dissolution behavior and pharmacokinetics of sulfasalazine pellets and spheroids. Dual-layer coating of sulfasalazine pellets, containing outer pH-dependent coating and inner microbiota-activated layer showed minimal drug release under simulated conditions of stomach and small intestine with subsequent controlled release of the drug in the colon. Combination with probiotics increased colon specificity of drug release and pharmacokinetics compared with conventional sulfasalazine administration. Variability of colonic pH and microbiota, lack of in-vitro-in-vivo correlation and clinical trials are important limitations. Use of pH-dependent and microbiota-activated coating systems can help to increase colon-targeting property of the drug, enhance its distribution in gastrointestinal tract and prevent dose dumping as compared to tablets.

Keywords: Sulfasalazine; Ulcerative colitis; Colon-targeted drug delivery; Multiparticulate pellets; Extrusion-spheronization; pH-dependent coating; Microbiota-triggered release; Eudragit; Guar gum; Pectin.

A Network Pharmacology Approach for the Exploration of the Therapeutic Potential of Pemafibrate in Parkinson's Disease

Shirit Agrawal*, Dr. Archana Navale
Department of Pharmacology, Parul Instituite of Pharmacy, Parul University, Vadodara, Gujarat, India
Shirit2805agrawal@gmail.com

ABSTRACT

Parkinson's disease (PD) is a progressive neurodegenerative disorder and loss of dopaminergic neurons is a key feature, with mitochondrial dysfunction, oxidative stress, and neuroinflammation all being key factors in the disease. Pemafibrate, a selective PPARα modulator, could act on molecular pathways that are involved in PD but the mechanism of action is not known. To use network pharmacology to find potential therapeutic targets and signaling pathways corresponding to the effects of pemafibrate in PD. Targets associated with Pemafibrate were extracted from publicly available databases and targets associated with PD were extracted from disease databases. Target proteins were defined and a protein–protein interaction network was created. Network Topology analysis was employed to identify hub genes, and then Gene Ontology (GO) and (KEGG) enrichment analysis was performed. The integrated network identified multiple common targets that connected pemafibrate and mechanisms of PD. A hub-target analysis identified proteins that are related to the metabolic regulation, oxidative stress, inflammation, and mitochondrial homeostasis. GO enrichment revealed that they were involved in cellular metabolism, response to oxidative stress, and molecular signaling. Although the pathways were not identified, KEGG analysis showed an enrichment of signaling via the EGFR, lipid metabolism, oxidative stress and mitochondrial pathways. The obtained indicate potentially neuroprotective activity of pemafibrate due to its multi-target activity on metabolic pathways, mitochondrial homeostasis and modulation of oxidative and inflammatory processes.

Keywords: Parkinson's disease, Pemafibrate, Network pharmacology, EGFR, Mitochondrial dysfunction, Oxidative stress, KEGG.

Overcoming Delivery Limitations of Sorafenib Using a PEGylated Liposomal System

Suraj Anand Priyadarshi[1]*, Dr. Avinash Pawar[1]
[1]Department of Pharmaceutics, School of Pharmacy, Parul University, Vadodara, Gujarat, India
anandsuraj4567@gmail.com

ABSTRACT

Sorafenib Tosylate (SRT) is a multikinase inhibitor with potential application in triple-negative breast cancer (TNBC). However, its therapeutic utility is limited by poor aqueous solubility, low and variable bioavailability, rapid systemic clearance, and dose-limiting toxicity. A PEGylated liposomal system was therefore explored to improve the delivery and performance of SRT. SRT-loaded PEGylated liposomes containing DSPG, egg-lecithin, cholesterol, and DSPE-mPEG-2000 were prepared by thin-film hydration and optimized using a Box-Behnken design. Lipid extrusion through 200 and 100 nm polycarbonate membranes was used to obtain uniform nanosized vesicles. The optimized formulation was evaluated for vesicle size, PDI, zeta potential, entrapment efficiency, solid-state characteristics, in vitro drug release, cytotoxicity and cellular responses in MDA-MB-231 cells, hemocompatibility, stability, pharmacokinetics, biodistribution, and tissue safety. The optimized PEGylated liposomes showed a vesicle size of 104.5 ± 4.0 nm, PDI of 0.097 ± 0.004, and entrapment efficiency of 82.5 ± 2.2%. Encapsulation converted SRT from its crystalline to amorphous form. The formulation provided sustained drug release, with 70.9 ± 4.9% released over 48 h compared with 96.8 ± 3.1% release from free SRT within 12 h. In MDA-MB-231 cells, IC50 decreased from 35.63 ± 4.6 to 18.25 ± 1.8 µg/mL, with increased cellular uptake, ROS generation, and mitochondrial depolarization. Hemolysis remained below 5%. In rats, the formulation increased plasma half-life by approximately 5.6-fold and AUC by approximately 10.8-fold, with reduced organ accumulation and no significant histopathological toxicity. PEGylated liposomal encapsulation addressed important delivery limitations of sorafenib by providing sustained release, enhanced anticancer activity, prolonged systemic exposure, and favorable safety characteristics. The optimized system demonstrates potential as a nanocarrier strategy for improving sorafenib delivery in TNBC.

Keywords: Sorafenib Tosylate; PEGylated liposomes; drug delivery; triple-negative breast cancer; lipid extrusion

Molecular Docking and Qsar Studies Of Novel Thiazolidinediones As Peroxisome Proliferator - Activated Receptor- γ Activator

Dr. Rupali Yevale
Associate Professor, Pharmaceutical Chemistry Department, K.G Rahul Dharkar College of Pharmacy and Research Institute, Karjat. Maharashtra, India.
rupaliyevale05@gmail.com

ABSTRACT

Computer-aided drug design methods were employed to investigate and optimize thiazolidinedione (TZD) derivatives targeting PPAR-γ. The three-dimensional structure of PPAR-γ (PDB 2PRG) was obtained from the Protein Data Bank and prepared for molecular docking. The binding site was defined with reference to the interactions observed between the receptor and its co-crystallized ligand, rosiglitazone, with particular attention to the hydrophobic regions known to accommodate ligand substituents. The proposed compounds were constructed as two-dimensional structures, converted into three-dimensional conformations, and subjected to energy minimization using VLife MDS v4.6. Molecular docking was subsequently performed using the Genetic Algorithm–based iGEM docking protocol in VLife, with a population size of 200 and 70 generations, while three docking solutions were retained. AutoDock Vina 1.2 was additionally employed as an independent docking method for comparison and validation. The resulting ligand receptor complexes were examined using UCSF Chimera 1.15 to characterize binding orientations and receptor–ligand contacts. Particular emphasis was placed on identifying important amino-acid residues, features of the binding pocket, and how changes in substituents and functional groups at different positions of the TZD scaffold influenced predicted affinity and selectivity for PPAR-γ relative to PPAR-α. The compound dataset was also divided into structurally diverse training and test subsets for the development of quantitative structure–activity relationship models. The 2D-QSAR analysis incorporated molecular, topological, and physicochemical descriptors, whereas the 3D-QSAR approach examined spatial and steric characteristics associated with biological activity. These models were used to investigate relationships between molecular structure and IC 50 values. Collectively, the docking, molecular visualization, ligand optimization, and QSAR analyses provided a computational framework for examining TZD derivatives and identifying structural features potentially associated with selective PPAR-γ agonist activity.

Computer-Aided Drug Design for Precision Medicine A Molecular Approach to Personalized Therapeutics

Chirag Aggarwal*, Navan Garg
Research Scholar, PCTE Group of Institute, Ludhiana, Punjab, 142021
1305chirag@gmail.com

ABSTRACT

Precision medicine is transforming drug discovery by enabling the development of therapies tailored to specific molecular, genetic, and biological characteristics of patients and disease subgroups. Computer-Aided Drug Design (CADD) plays a significant role in this approach by providing computational tools to identify, evaluate, and optimize potential drug candidates against specific biological targets. Molecular docking and virtual screening facilitate the identification of compounds with favourable interactions with disease-associated proteins, while quantitative structure–activity relationship (QSAR) modelling supports the prediction of biological activity from molecular properties. Molecular dynamics simulations provide additional insights into the stability and behaviour of drug–target complexes. Furthermore, ADMET and drug-likeness prediction enable the early assessment of pharmacokinetic and safety-related properties, supporting the selection of suitable candidates before extensive experimental studies. The integration of artificial intelligence and machine learning has further strengthened CADD through molecular property prediction, large-scale screening, and optimization of drug candidates. These computational approaches can contribute to more rational, efficient, and targeted drug discovery by integrating molecular information with predictive modelling. However, challenges related to data quality, model reliability, biological complexity, and experimental validation remain important. Therefore, the greatest potential of CADD in precision medicine lies in an integrated computational and experimental framework. Overall, the combination of precision medicine and CADD offers a promising strategy for developing more targeted, effective, and potentially safer therapeutic interventions.

Keywords: Precision Medicine, Computer-Aided Drug Design, Molecular Docking, Virtual Screening, QSAR, ADMET, Artificial Intelligence, Drug Discovery.

Digital Twin-Assisted Personalized Drug Discovery Convergence of Artificial Intelligence, CADD and Computational Pharmacology

Araki Esam*, Navan Garg
Research Scholar, PCTE Group of Institutes, Ludhiana, Punjab, 142021
arakiesam7@gmail.com

ABSTRACT

The increasing complexity of human diseases and variability in individual drug responses have created a growing need for personalized approaches to drug discovery and development. Digital twin technology provides a promising framework for developing computational representations of patients, organs, biological systems, and disease processes by integrating clinical, molecular, physiological, and pharmacological data. This review examines the integration of digital twins with artificial intelligence (AI), computer-aided drug design (CADD), and computational pharmacology for personalized therapeutic discovery. Key computational approaches, including molecular docking, virtual screening, quantitative structure–activity relationship modelling, molecular dynamics simulations, pharmacokinetic and pharmacodynamic modelling, and AI-based predictive analytics, are evaluated within the digital twin framework.The convergence of these technologies enables the integration and interpretation of complex biological datasets to support target identification, candidate molecule evaluation, and prediction of molecular interactions. Digital twin-assisted platforms may facilitate virtual testing of therapeutic candidates, prediction of patient-specific drug responses, optimization of dosing strategies, and early identification of potential toxicity or treatment failure. Computational pharmacology further supports modelling of drug absorption, distribution, metabolism, excretion, pharmacodynamics, and dose–response relationships, while AI improves data analysis and predictive modelling. The integration of AI, CADD, computational pharmacology, and digital twin technology represents a promising approach toward more efficient, predictive, and personalized drug discovery. However, challenges involving data quality, biological complexity, model validation, interoperability, privacy, and regulatory acceptance must be addressed. Digital twin-assisted drug discovery should therefore complement, rather than replace, experimental and clinical investigations, providing an integrated framework for precision therapeutic development.

Keywords: Digital Twin, Personalized Drug Discovery, Artificial Intelligence, Computer-Aided Drug Design, Computational Pharmacology**.**

Gastro-Protective Live Probiotic Nano-carriers A Review of a Novel Gut Brain Axis Strategy for Alzheimer's Disease

Anant Pai[1], Shraddha Patel*, Archana Navale*
Department of Pharmacology, Parul Institute of Pharmacy, Parul University, Vadodara (391760), Gujarat, India
anantpai2702@gmail.com

ABSTRACT

Alzheimer's disease (AD) is chronic progressive neurodegenerative disorder characterized by dementia and it has no disease modifying treatment. Gut microbiota plays a key role in its pathology. Live probiotics showed neuroprotective potential in preclinical AD models, but gastric acid destroy bacterial viability before colonic colonization, limiting oral delivery. This review examines whether nanocarrier encapsulation can overcome this limitation for AD targeted probiotic therapy. A structured literature review was conducted using Scopus, PubMed, and Google Scholar (2016-2025), using combined search terms including "Probiotics and Alzheimer's disease," "Gut-Brain-Axis and Neuroinflammation," "pH-responsive nanocarrier and Gastric Protection," "Akkermansiamuciniphila and Amyloid beta," and "PLGA/chitosan nanoparticles and oral delivery." Peer-reviewed preclinical in-vivo studies were included if they discussed gut microbiota-AD interactions, probiotic efficacy in transgenic AD models or nanocarrier based gastrointestinal/ BBB delivery systems. Non-peer-reviewed sources and AD-unrelated studies were excluded. Selected evidence was organized in four mechanistic domains restoration of microbiota, intestinal barrier integrity, immune modulation and neuroprotection. Rather than replicating findings from earlier single-domain reviews, this review reveals a previously unexplored connection probiotic strains such as Akkermansiamuciniphila and Lactobacillus/Bifidobacterium are independently validated for reversing AD associated cognitive and neuroinflammatory changes, and independently validated for gastric survival and brain-targeted release of small molecule like curcumin, yet no existing study unites the two. This review proposes, for the first time, a conceptual gastro-protective delivery for viable AD relevant probiotic strains rather than small molecule as a mechanistically justified but untested therapeutic direction. The efficacy of probiotics in AD and nanocarrier based gastric protection are independently validated but never integrated. This review's novel contribution is bridging these two domains into a single translational hypothesis; in vivo validation of live probiotic nano-encapsulation could represent one of the promising approach for the management of AD.

Keywords: Alzheimer's Disease, Gut Microbiota, Nanocarrier, Live Probiotics.

Modern Computer-Aided Drug Design Tools in Drug Discovery from Target Identification to Lead Optimization

Ruchita Sharma*, Dr Nidhi Namdev
G.R.Y. Institute Of Pharmacy, Borawan
ruchitasharma623@gmail.com

ABSTRACT

Computer-Aided Drug Design (CADD) has emerged as a powerful approach for accelerating modern drug discovery by reducing the time, cost, and resources required for conventional experimental methods. CADD integrates computational techniques to identify promising drug candidates and optimize their pharmacological properties at an early stage of development. Structure-based and ligand-based approaches, including molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulation, quantitative structure–activity relationship (QSAR), and in-silico ADMET prediction, enable researchers to investigate drug–target interactions and predict the behavior of potential therapeutic molecules. Several computational tools, such as AutoDock Vina, PyRx, SwissADME, Chimera, ChemDraw, and Discovery Studio, facilitate ligand preparation, molecular visualization, docking analysis, and drug-likeness assessment. The integration of artificial intelligence and machine learning with CADD is further enhancing target identification, hit discovery, lead optimization, and prediction of pharmacokinetic and toxicity profiles. By enabling the rapid screening of large chemical libraries and prioritizing molecules with desirable biological properties, CADD provides a rational and efficient pathway for drug development. This presentation highlights major CADD tools, their principles, applications, advantages, limitations, and their role in transforming conventional drug discovery into a more predictive, data-driven, and efficient process.

Keywords: Computer-Aided Drug Design; Molecular Docking; Virtual Screening; ADMET Prediction.

Multifaceted Application of GLP-1 Receptor Agonists in Modern Medicine

Diya Patel*, Dr. Navdha Vyas, Dr. Shraddha Patel,
Department of Pharmacology, Parul Institute of Pharmacy, Parul University, Vadodara, Gujarat
diya.m1508@gmail.com

ABSTRACT

GLP-1 receptor agonists (GLP-1RAs), derived from the incretin hormone GLP-1, have emerged from being just glucose-lowering drugs to being multi-targeted drugs. These agents have pleiotropic actions that have nothing to do with glycemic control; they are broadly distributed in the pancreas, gastrointestinal tract, heart, kidney, liver, immune system and central nervous system. Although they are increasingly used in clinical practice, a comprehensive knowledge of their mechanisms in various organ systems is still required. This review represents how GLP-1 can have multiple effects and the emerging potential for therapy, including its physiological role, classification and molecular mechanisms in the cardiometabolic, renal, hepatic, immune and neurological systems.The literature referenced in this narrative was critically reviewed from recently published, peer-reviewed publications in high-impact journals covering aspects of the origin, secretion, classification, and receptor pharmacology of GLP-1 and mechanistic and clinical outcome information for GLP-1RAs in the cardiovascular, renal, hepatic, neurodegenerative, and immune-related disease arena.GLP-1RAs improve glucose-dependent insulin secretion, inhibit glucagon, slow gastric emptying and cause satiety.There are also nephroprotective and hepatoprotective effects, such as decreased albuminuria, slowing the decline in eGFR, reduced lipogenesis, improvement of insulin sensitivity, and decreased hepatic steatosis and inflammation in MASH/NASH. There is emerging evidence for neuroprotective effects, including anti-accumulation of amyloid-β and α-synuclein, anti-neuroinflammation and anti-mitochondrial dysfunction; these effects are expected to be beneficial in Alzheimer's and Parkinson's disease. Anti-inflammatory and immunomodulatory effects of GLP-1RAs also include a reduction in the release of pro-inflammatory cytokines from T cells and macrophages.GLP-1RAs are pleiotropic agents that act on interconnected pathways of the cardiometabolic, renal, hepatic, immune and neuronal systems.

Keywords: GLP-1 receptor agonists, Pleiotropic effects, Cardio protection, Neuroprotection, Hepatoprotection, Nephroprotection, Precision Medicine.

Structure-Based Drug Design (SBDD)

Mr. Monesh Kushwaha*
SBS Daddu Ji College Of Pharmacy (MajorSD Singh University), Farrukhabad
Kmonesh55@gmail.com

ABSTRACT

Structure-Based Drug Design (SBDD) is the process of designing and optimizing drugcandidates using the three-dimensional structure of a biological target to predict and improve molecular interactions between the drug and its target. It is a modern computational drug discovery approach in which the three-dimensional (3D) structure of a biological target (such asa protein, enzyme, or receptor) is used to design and optimize drug molecules. The target structure is usually determined by X-ray crystallography, Nuclear Magnetic Resonance (NMR) spectroscopy, or Cryo-Electron Microscopy (Cryo-EM).Disease Selection → Target Identification → Target Validation → Determination of 3D Structure (X-ray Crystallography / NMR / Cryo-EM) → Protein Preparation → Active Site Identification → Ligand Preparation → Virtual Screening → Molecular Docking → Binding Energy & Interaction Analysis → Lead Identification → Lead Optimization → ADMET Prediction → Molecular Dynamics Simulation → In-vitro Evaluation → In-vivo Evaluation → Clinical Trials → Drug Approval.The Result of Structure-Based Drug Design (SBDD) is the identification and development of a safe, effective, selective, and optimized drug candidate that binds strongly to the target protein and exhibits desirable pharmacological and pharmacokinetic properties. Through computational techniques such as virtual screening, molecular docking, molecular dynamics simulation, onlythe most promising compounds are selected for experimental testing. These lead molecules are then validated through in vitro or in vivo studies, and clinical trials**.** **I**t is a powerful and rational approach to modern drug discovery that uses the three-dimensional structure of biological targets to design and optimize drug molecules. By integrating computational tools with experimental validation.

Keywords: Structure-Based Drug Design (SBDD), Computer-Aided Drug Design (CADD), Three-Dimensional (3D) Protein Structure, Biological Target, Drug Target, Protein Structure.

Systems Biology and Network Pharmacology Approach to Statin-Induced Coenzyme Q10 Deficiency Insights into Lipid Crosstalk, TNF–MAPK Signaling, and Myotoxicity

Nila Ganamurali[1], Sarvesh Sabarathinam[2]
Helix Research Studio, Saveetha Medical College and Hospital, Saveetha Institute of Medical and Technical Sciences, Saveetha Nagar, Thandalam, Chennai - 602105, Tamil Nadu, India
nilaganamurali@gmail.com

ABSTRACT

Statin-associated muscle symptoms (SAMS) remain a major reason for treatment discontinuation, and Coenzyme Q10 (CoQ10) depletion from mevalonate pathway inhibition is a suspected contributor. The molecular links between CoQ10 deficiency and muscle symptoms are not well defined. Gene targets for SAMS, CoQ10 deficiency, and statins were collected from GeneCards, and overlapping genes were mapped using STRING protein–protein interaction analysis. Hub genes were identified with CytoHubba, and ShinyGO was used for pathway enrichment.145 genes were shared across the three datasets, with strong enrichment in inflammatory, metabolic, and mitochondrial pathways. TNF appeared as the top hub gene, linked to MAPK-driven apoptotic and stress-response signaling. The resulting network suggests that statin-mediated mevalonate pathway suppression lowers CoQ10 synthesis, which sensitizes muscle to cytokine-driven inflammation and raises apoptotic vulnerability. These point to mitochondrial dysfunction, oxidative stress, and disrupted energy metabolism as downstream effects of CoQ10 loss in SAMS, with the TNF–MAPK axis acting as a central mechanistic link between immune activity, lipid metabolism, and mitochondrial health. The findings offer a molecular basis for interventions such as CoQ10 supplementation or anti-inflammatory approaches, though experimental and clinical studies are needed to confirm these computational predictions.

Keywords: Statin-associated muscle symptoms; Coenzyme Q10; network pharmacology; TNF; MAPK signaling; mitochondrial dysfunction

Wearable Devices for Diabetes Emerging Trends in AI Integration and Multi-Biomarker Approaches

Mr. Krishnendu Ghosh[1*], Dr. Ahana Hazra[1], Dr. Mithun Bhowmick[1]
[1]Bengal College of Pharmaceutical Sciences and Research, Durgapur, 713212, West Bengal, India
krishnendu.ghoshdgp@gmail.com

ABSTRACT

Diabetes mellitus is a chronic metabolic disorder that requires continuous monitoring and effective management to prevent severe complications such as cardiovascular diseases, neuropathy, nephropathy, and retinopathy. Recent advancements in wearable sensing technologies, combined with artificial intelligence (AI), have transformed diabetes care by enabling real-time, personalized, and data-driven health monitoring. AI-integrated wearable devices utilize electrochemical, optical, microneedle, sweat-based and smart contact lens sensors to continuously measure glucose levels and other physiological parameters with minimal or no invasiveness. It helps to predict glucose fluctuations, detect abnormalities, and provide personalized therapeutic recommendations. The convergence of AI and wearable multi-biomarker technologies represents a promising paradigm for precision diabetes management, offering improved patient outcomes, enhanced quality of life, and more efficient healthcare delivery. Additionally, integrating these technologies into existing healthcare systems requires proper regulatory frameworks, infrastructure, and training for healthcare professionals.AI-integrated wearable technologies offer a promising approach to personalized diabetes management through continuous monitoring, glucose prediction, automated insulin delivery, and remote healthcare. Additionally, integrating these technologies into existing healthcare systems requires proper regulatory frameworks, infrastructure, and training for healthcare professionals.

Keywords: Diabetes Mellitus, Remote Patient Monitoring, Mobile Health (mHealth), Wearable Devices, Smart Insulin Pumps, Microneedle Sensors

E-Pharmacy and Online Drug Distribution

[1]Poonam Kaimaiyan,
Dr. Anar Singh College of Pharmacy,(Major SD Singh University) Farrukhabad
p.kaimaiyan@gmail.com

ABSTRACT

Online pharmacy" (Internet or mail-order pharmacy) is an umbrella term for retailers of non-prescription and prescription medicines that dispense or sell medicines directly to patients through the mail and provide information on their products and services via the internet. It is important to delineate the types of online pharmacies that have been identified in the published literature. These include chain pharmacies that operate online, online pharmacies that operate solely online, and brick-and-mortar pharmacies that have an online presence. Consumers may choose to utilise online pharmacies for a multitude of reasons, such as convenience, 24/7 accessibility, price transparency, potentially greater consumer privacy and availability of products.E-pharmacyis anonlinepharmacythatoffers convenient, cost-effective,androundthe-clock access to medicines, driven by e-prescriptions and the COVID-19 pandemic.cross-sectional questionnaire-based study was conducted among Compulsory Rotatory Medical Interns (CRMIs) to assess their awareness and knowledge regarding E-pharmacy. A structured questionnaire covering the concept, advantages, legal status, safety concerns, prescription requirements, and risks associated with online medicine purchasing was prepared.The study showed that CRMIs had moderate awareness regarding E-pharmacy, but gaps were observed in their knowledge of legal regulations, patient safety, prescription requirements, and risks associated with purchasing medicines online.Thestudyconcludesthat CRMIs have awareness about E-pharmacy,but gaps exist in knowledge regarding its legal, safety, and regulatory aspects.

Keywords: E-Pharmacy, Patient Safety, Drug safety, online pharmacy regulation, Accessibility (24/7 Healthcare Access) and awareness of E-Pharmacy.

Evaluation of Histopathological and Fibrotic Biomarker Changes in Arecoline-Induced Oral Submucous Fibrosis in Rats

[1]Sweta Rana, [2]Nikhil Kumar
Department of Pharmacology, Parul Institute of Pharmacy, Parul University, Gujarat, India
swetarana032@gmail.com

ABSTRACT

Oral submucous fibrosis (OSMF) is a chronic, potentially malignant disorder of the oral cavity strongly associated with areca nut chewing. Arecoline, the principal alkaloid in areca nut, is implicated in inducing fibroblast proliferation and excessive collagen deposition, leading to progressive submucosal fibrosis. This study aimed to evaluate histopathological and fibrotic biomarker changes in an arecoline-induced rat model of OSMF.Wistar rats were divided into a normal control group and an arecoline-induced model group. The model group received submucosal buccal injections of arecoline hydrochloride (2 mg/mL), administered three times weekly for a period of 8–16 weeks. Mouth-opening measurements were recorded to assess trismus. Buccal mucosal tissue was examined histopathologically using Hematoxylin and Eosin staining and graded per the Pindborg–Sirsat classification. Oxidative stress markers were assessed, and immunohistochemical analysis for Collagen I, Collagen III, and TGF-β1 expression was performed to evaluate fibrotic activity. Arecoline-treated rats showed a significant, time-dependent reduction in mouth opening compared to controls. Histopathological examination revealed progressive juxta-epithelial fibrosis, epithelial atrophy, and reduced vascularity consistent with advancing Pindborg–Sirsat grades. Immunohistochemistry demonstrated markedly increased expression of Collagen I, Collagen III, and TGF-β1 in the model group, alongside elevated oxidative stress marker levels, correlating with the severity of fibrosis. Chronic arecoline exposure induces histopathological and molecular changes closely resembling human OSMF, with TGF-β1-mediated collagen deposition playing a central role in disease progression. This model supports arecoline's causative role in OSMF and provides a platform for evaluating future therapeutic interventions.

Keywords: Areca nut, Arecoline, Oral submucous fibrosis, TGF-β1, Collagen, Fibrosis

Exploring The Immuno Stimulant Potential Of*dryopteris Cochleata* An Insilico Approach

Shubhangi Patil[1]*, Popat Kumbhar[2], John Disouza[3]

1. Department of Pharmaceutics, KCT'sKrishna College of Pharmacy, Karad,415539
2. Department of Pharmaceutics, Tatyasaheb Kore College of Pharmacy, Warana University,
3. Bombay Institute of Pharmacy & Research, Dombivli, Mumbai, Maharashtra, India,421204

patil.shubhangi13@gmail.com

ABSTRACT

Chronic inflammation is a hallmark of several autoimmune and inflammatory disorders, including psoriasis, rheumatoid arthritis, inflammatory bowel disease, and diabetes mellitus. Pro-inflammatory cytokines such as interleukin-1β (IL-1β), interleukin-6 (IL-6), and interferon-gamma (IFN-γ) play crucial roles in the initiation and progression of inflammatory responses, making them attractive therapeutic targets. The structures of IL-1β (4DEP), IL-6 (1ALU), and IFN-γ (1FG9) were obtained from the RCSB Protein Data Bank and refined using the Schrödinger Protein Preparation Wizard. Docking studies were performed using Glide Standard Precision. Swiss ADME was used to predict drug like properties and pharmacokinetics. Stability of chosen protein-ligand complexes was assessed by 100 ns Desmond molecular dynamics simulations with RMSD, RMSF, Rg, SASA, PCA and FEL analyses. Molecular docking has shown Quercetin, Gibberellin A3, and Aspidinol as promising ligands for IL-6. Gibberellin A3 showed the best binding to IL-1β, and of thethree, Ferulicacidshowedthehighestaffinityto IFN-γ. Quercetinhadthe best IL-6dockingscore (−6.522kcal/mol), andGibberellinA3hadthebestIL-1βbinding (−6.866 kcal/mol), both scores were greater than levamisol. Computational analyses identified Aspidinol and Gibberella A3 fromDryopteris cochleata as having good immunomodulatory potential because of favorable cytokine binding and good pharmacokinetics. This requires further in vitro and in vivo validation to confirm their therapeutic potential.

Keywords: Molecular docking; Molecular dynamics simulation; Swiss ADME; BOILED-Egg model; IL-1β; IL-6; IFN-γ.

Development and Evaluation of Quetiapine Fumarate-Loaded Transferosomal Intranasal i*n Situ* Gel for Brain Targeting in Schizophrenia

Talati Jeet[1], Nafisha Abdal[1], Meenakshi B. Patel[1]
[1]Department of Pharmaceutics, School of Pharmacy, Faculty of Pharmacy, Parul University, Waghodia, Vadodara – 391760, Gujarat, India
2508422110013@paruluniversity.ac.in

ABSTRACT

Quetiapine fumarate (QTF), a second-generation atypical antipsychotic, is used to treat schizophrenia; however, its oral bioavailability is limited (9%) due to low solubility and extensive first-pass metabolism. Intranasal drug delivery offers a non-invasive approach for direct nose-to-brain transport, bypassing the blood–brain barrier and hepatic metabolism. Transferosomes, owing to their ultra-deformable nature, enhance drug permeation, while incorporation into an ion-sensitive in situ gel prolongs nasal residence time and sustains drug release. Transferosomes were prepared using the thin-film hydration method and optimized using a Box–Behnken design, with phospholipid concentration, cholesterol concentration, and sonication time as independent variables. The optimized formulation was incorporated into an ion-sensitive in situ gel containing deacylated gellan gum and HPMC. The formulation was evaluated for vesicle size, polydispersity index (PDI), zeta potential, entrapment efficiency, in vitro drug release, ex vivo permeation, release kinetics, and stability. The optimized formulation exhibited a vesicle size of 97 ± 2.1 nm, PDI < 0.3, zeta potential of −20 ± 1.8 mV, and 77.5 ± 2.4% entrapment efficiency. FTIR, DSC, and XRD confirmed the absence of drug–excipient interactions and indicated partial amorphization of QTF. TEM revealed spherical nanometric vesicles. The formulation showed sustained in vitro drug release (70.2% at 480 min) compared to the pure drug (58.4%) and enhanced ex vivo permeation (77%). The transferosomal intranasal in situ gel demonstrated improved drug release, enhanced nasal permeation, and potential for direct nose-to-brain delivery. These findings suggest that the proposed system is a promising strategy for improving the therapeutic efficacy of QTF in schizophrenia.

Keywords: Quetiapine fumarate, Transferosomes, Intranasal delivery, In situ gel, Nose-to-brain delivery, Schizophrenia.

Formulation Development and Evaluation of Raloxifene Hydrochloride Tablets for Enhanced Drug Release

Monil Sisotia, Bhushan Vasant Patil, Dr. Rajesh Dodiya
Department of pharmaceutics, school of pharmacy, faculty of pharmacy, parul university
Waghodia, vadodra – 391 760 gujrat, india
2508422110010@paruluniversity.ac.in

ABSTRACT

Raloxifene Hydrochloride (RLX) is a selective estrogen receptor modulator (SERM) widely used in managing postmenopausal osteoporosis. However, its clinical efficacy is constrained by low oral bioavailability (~2%), driven by poor aqueous solubility (BCS Class II) and extensive first-pass metabolism. This study aimed to enhance the dissolution rate and oral bioavailability of RLX by formulating solid dispersion-based tablets optimized via a 3^2 full factorial design. Preformulation studies included melting point determination, UV-Vis spectrophotometry (λ_{max}=288 nm), and FTIR spectroscopy. Solid dispersions were prepared by solvent evaporation and melting methods using hydrophilic carriers. The dispersions were blended with excipients (MCC, Ac-Di-Sol, PVP K30, Magnesium Stearate) and compressed into tablets via wet granulation. Pre-compression flow parameters and post-compression properties were thoroughly evaluated. FTIR spectra revealed no chemical interaction between RLX and the carriers. Increasing carrier proportions enhanced drug solubility, while higher levels of the superdisintegrant Ac-Di-Sol reduced tablet disintegration time to approximately 3.5 minutes. Optimized tablets exhibited satisfactory pre-compression flow properties, low friability (<1%), uniform weight distribution, rapid disintegration, and markedly accelerated *in vitro* drug release profiles. Overall, solid dispersion using hydrophilic carriers like PEG 4000 and Urea successfully overcomes the solubility limitations of RLX, presenting a viable formulation strategy for enhanced oral drug delivery.

Keywords: Raloxifene Hydrochloride, Solid Dispersion, Solubility Enhancement, PEG 4000, Factorial Design

Unlocking the Therapeutic Potential of Momordica charantia Linn. From Traditional Use to Modern Drug Discovery

Ketaki Shinde *
Research Scholar, Department of Pharmaceutical Sciences, Krishna Institute of Pharmacy, Krishna Vishwa Vidyapeeth (Deemed to be University), Karad - 415539, Maharashtra, India.
jkomal2442@gmail.com

ABSTRACT

Momordica charantia Linn., commonly known as bitter melon or bitter gourd, is an important medicinal plant extensively used in traditional Asian medical systems for the prevention and management of various diseases. This review aims to compile and critically summarise updated information on its phytochemistry, pharmacological activities, toxicological profile, ethnomedicinal uses, and commercial and phytopharmaceutical relevance.A comprehensive literature survey was conducted using English-language publications, focusing on pharmacological evaluations, isolation and characterisation of bioactive compounds, toxicological studies, and both traditional and modern applications of M. charantia.Pharmacological investigations have demonstrated a wide range of bioactivities, including hepatoprotective, cardioprotective, and anti-inflammatory effects, as well as other therapeutic effects, from extracts of different plant parts. Numerous bioactive constituents have been identified, such as triterpenes, proteins, steroids, alkaloids, lipids, inorganic components, and phenolic compounds. Several novel molecules, including kuguacin-J, momordicine-I, α-eleostearic acid, momordicoside A, quercetin-3-O-glycoside, cucurbitacin E, and goyaglycoside-G, exhibit significant therapeutic potential. The review also highlights traditional and contemporary uses, phytopharmaceutical formulations, toxicity considerations, and other applications. Despite its long-standing traditional use, many therapeutic claims remain scientifically unvalidated, emphasising the need for further mechanistic and clinical studies to identify active principles and their synergistic effects.

Keywords: Momordica charantia Linn., Pharmacological Activity, Phytochemistry, Phytopharmaceutical Formulation, Toxicity, Traditional Medicinal Uses.

Development and Evaluation of Chitosan-CoatedAprepitant-Loaded Nanoparticles for Breast Cancer

Kashish Joshi[a], Ekta Pardhi[a], Rahul Khemchandani[b], Neelesh Kumar Mehra[a], Avinash Pawar[a], Gananadhamu Samanthula[a], Tanmoy Chatterjee[c*]

[a]*Department of Pharmaceutics, National Institute of Pharmaceutical Education and Research, Hyderabad, India,* [b]*Department of Pharmaceutical Analysis, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India,* [c]*Parul University*

*2508422110014@paruluniversity.ac.in / avinash.pawar44040@paruluniversity.ac.in

ABSTRACT

Breast cancer remains a major global health burden, and resistance plus metastasis still limit current treatments. The paper focuses on NK-1 receptor signaling and the anticancer potential of aprepitant, but notes its poor solubility and bioavailability, motivating nanoparticle-based delivery.The researchers prepared aprepitant-loaded BSA nanoparticles by the desolvation method, coated with chitosan, and optimized the formulation using Box-Behnken design under Quality-by-Design approach.They characterized the nanoparticles using DLS, TEM, FTIR, DSC, PXRD, NMR, release studies, hemolysis tests, docking, and cell-based assays.The optimized CS-APT-BSANPs had a particle size of about 160 nm, PDI of 0.211, zeta potential of 31 mV, and entrapment efficiency of 87.0%. They showed stronger cytotoxicity than free aprepitant, improved cellular uptake, apoptosis, caspase-3 activation, better tumor penetration.CS-APT-BSANPs were shown to be stable, biocompatible, and effective for targeted aprepitant delivery in breast cancer. The study concludes that this protein–polymer hybrid nano-system can improve therapeutic efficacy by enhancing solubility, release behavior, and anticancer activity.

Keywords: Aprepitant, breast cancer, chitosan-coated BSA nanoparticles, Dynamic Light Scattering (DLS), Differential Scanning Calorimetry. Cell line study.

Formulation And Evaluation of Posaconazole-Loaded Niosomal Gel For Topical Treatment Of Cutaneous Candidiasis

Tejas Ranpara, Isha Patel, Khushboo Kathrotiya, Meenakshi. Patel
Department of Pharmaceutics, Faculty of Pharmacy, School of Pharmacy, Parul University–Waghodia, Vadodara - 391760
meenakshi.patel24771@paruluniversity.ac.in

ABSTRACT

The Cutaneous candidiasis refers to the infection of the skin with candida fungus. To ensure good treatment, it requires excellent topical formulations capable of effectively delivering the drug to skin. This research was aimed to design, optimize, and characterize a new type of "niosomal gel" of posaconazole, a novel antifungal agent, to facilitate topical delivery of posaconazole and enhance its efficacy against various fungi. A novel film hydration technique was used to synthesize tiny, drug-laden niosomeusingSpan 80, Tween 80 and cholesterol. The niosome were blended in a Carbopol 934 gel base. To achieve the desiredparticle size andmaximum loading of the drug, a 3^2 factorial experimental design was applied and the quantities of the surfactantsandcholesterolwere varied to optimize the formula. The most suitable formulation (F8) was able to yield stable nanoparticles (156.4 nm) with acceptable drug loading and entrapment efficiency (68.4%). This formulation also demonstrated acceptable skin friendliness, such as appropriate skin pH (5.53) and spreadability. Laboratory experiments revealed the sustainable release of drug from the niosomal gel as well as its improved deposition in the skin with compare to simple non-entrapped gel. Antifungal activity assay indicated higher inhibitory zone of niosomal gel against the Candida albicans growth (18.6 mm) in comparison to non-entrapped gel (12.4 mm). POS-Niosome-gel developed here clearly proved efficient in targeting the site of action & in enhancing the antifungal activity. This indicates that it may prove to be a viable &effective topical formulation for fungal infections of skin including cutaneous candidiasis.

Keywords: Posaconazole, Niosomalgel, Topical drug delivery, cutaneous candidiasis, thin film hydration method

Cinnamaldehyde-Rich Cinnamon Bark Extracts for Acne Vulgaris Mechanisms and Advanced Topical Delivery

Ishu Bhandari, IshuGarg*
College of Pharmacy, Shivalik Campus, Shimla Bypass Rd, Shiniwala, P.O. Sherpur, Dehradun-248197, Uttarakhand, India
ishabh1805@gmail.com

ABSTRACT

Acne vulgaris is a common multifactorial inflammatory skin disorder involving sebaceous hyperactivity, follicular hyperkeratinization, microbial dysbiosis, and persistent inflammation. The increasing antimicrobial resistance associated with prolonged use of topical antibiotics has stimulated interest in alternative, multi-target therapeutic approaches. Cinnamon bark, particularly *Cinnamomum verum* and *Cinnamomum burmannii*, is a promising phytotherapeutic source rich in cinnamaldehyde, a bioactive compound with reported antimicrobial, anti-inflammatory, antioxidant, and potential sebostaticproperties. This review explores the therapeutic potential of cinnamaldehyde-rich cinnamon bark extracts for acne management, with emphasis on their phytochemical profile, molecular mechanisms, and formulation strategies. The antimicrobial activity against acne-associated microorganisms, including *Cutibacterium acnes* and *Staphylococcus epidermidis*, together with modulation of inflammatory pathways such as NF-κB and COX-2, is discussed. The potential role of cinnamaldehyde in regulating oxidative stress and sebocyte activity is also highlighted. Furthermore, advanced topical delivery approaches, including nanoemulsions, liposomes, lipid nanoparticles, polymeric nanocarriers, hydrogels, and nanogels, are reviewed for improving stability, skin deposition, controlled release, and tolerability. The review also highlights key challenges, including extract standardization, variability in cinnamaldehyde content, formulation stability, skin irritation, and limited clinical evidence. Overall, cinnamaldehyde-rich cinnamon bark extracts represent a promising multi-target approach for acne management, warranting further standardized formulation development and well-designed clinical investigations.

Keywords: Acne vulgaris; Cinnamon bark; Cinnamaldehyde; Anti-inflammatory; Antimicrobial; Nanocarriers; Topical delivery

Smart Polymer-Based Transmucosal Patches for the Management of Oral Mucosal Injuries

Monika Gusain*, Ishu Garg
College of Pharmacy, Shivalik Campus, Shimla Bypass Rd, Shiniwala, P.O. Sherpur, Dehradun-248197, Uttarakhand, India
gusainmonika.05@gmail.com

ABSTRACT

Oral mucosal injuries, including traumatic lesions, aphthous ulcers, and postoperative wounds, present significant therapeutic challenges due to continuous salivary flushing, mechanical stress, microbial exposure, and rapid epithelial turnover. These factors limit the residence time and effectiveness of conventional formulations such as mouthwashes, gels, and ointments. Transmucosal patches offer an attractive alternative by providing prolonged mucosal residence, localized drug delivery, sustained release, and improved patient compliance. Recent advances in polymer science have enabled the development of smart polymer-based patches that respond to physiological stimuli such as pH, temperature, moisture, ionic strength, and enzymatic activity. This review critically examines the application of smart polymers in transmucosal patches for oral mucosal injury management, focusing on the relationship between polymer properties, stimulus responsiveness, mucoadhesion, mechanical performance, and drug-release behavior. Natural, synthetic, modified, and nanocomposite-based smart polymers are discussed, together with their applications in the localized delivery of antimicrobial, anti-inflammatory, analgesic, antioxidant, wound-healing, and biologic therapeutics. Available in vitro, ex vivo, in vivo, and clinical evidence is evaluated to highlight their therapeutic potential and translational relevance. Key challenges, including salivary interference, mucosal retention, mechanical stability, taste, patient acceptability, drug stability, manufacturing scalability, and regulatory considerations, are also addressed. Finally, emerging directions involving bioresponsive, multifunctional, personalized, and regenerative polymer platforms are discussed. Overall, smart polymers offer considerable potential for developing adaptive transmucosal patches that combine prolonged retention, controlled drug delivery, and enhanced mucosal healing.

Keywords: Oral mucosal injury; Transmucosal patches; Smart polymers; Stimuli-responsive polymers; Mucoadhesion; Controlled drug delivery; Wound healing; Oral drug delivery

Luteolin-Loaded Solid Lipid Nanoparticles Incorporated into a Thermosensitive In-Situ Gel for Localized Periodontal Drug Delivery

Sahana Narayana Harikantra[1], Dr. Hemanth Kumar S[2]
[1]Department of Pharmaceutics, Branch Quality AssuranceJSS College of Pharmacy, Mysuru, Karnataka, India
[2]Associate Professor, Department of Pharmaceutics, JSS College of Pharmacy, Mysuru, Karnataka, India
sahanaharikantra23@gmail.com

ABSTRACT

Periodontitis is a chronic inflammatory disease in which conventional treatment may be limited by inadequate drug concentration at the periodontal site, systemic adverse effects, and prolonged therapy. Luteolin, a naturally occurring flavonoid with anti-inflammatory, antimicrobial, and bone-regenerative properties, offers potential for localized periodontal treatment. The present study aimed to develop a luteolin-loaded solid lipid nanoparticle (LT-SLN) incorporated into a thermosensitive in-situ gel for sustained and localized drug delivery.LT-SLNs were prepared by high-shear homogenization followed by ultrasonication using Luteolin, Compritol 888 ATO, soy lecithin, and Tween 80. A Central Composite Design was employed using Design-Expert software to optimize formulation variables based on particle size, polydispersity index (PDI), and entrapment efficiency (EE). The optimized LT-SLNs were characterized by FT-IR, DSC, XRD, particle size, zeta potential, EE, SEM, TEM, and in-vitro drug release. The optimized nanoparticles were subsequently incorporated into a thermosensitive in-situ gel containing Poloxamer 407 and Carbopol 934 and evaluated for pH, syringe ability, gelation temperature, viscosity, drug release, sterility, and short-term stability. The optimized LT-SLN formulation showed a particle size of 234.6 nm, PDI of 0.039, and EE of 90%. The thermosensitive in-situ gel exhibited a gelation temperature of approximately 32.3°C, physiological pH of 7.2 ± 0.5, and suitable viscosity of 80.5 ± 5 cP. In-vitro release studies demonstrated sustained release of 99.23% from LT-SLNs over 120 hours and 99.65% from the in-situ gel over 144 hours. The formulation remained sterile and stable for 28 days. The developed luteolin-loaded thermosensitive in-situ gel demonstrated promising characteristics for sustained and localized periodontal drug delivery and may improve the therapeutic potential of luteolin in periodontitis management.

Keywords: Luteolin; Solid Lipid Nanoparticles; Thermosensitive In-situ Gel; Periodontitis; Sustained Drug Delivery.

Nanophytomedicine Through Green Synthesis Recent Advances, Biological Mechanisms, and Therapeutic Perspectives

Mr. Abushan Khan and Dr. Kaushal Kumar
Research Scholar, Department of Pharmacy, MJP Rohilkhand University, Bareilly, UP, 243006
*Associate Professor, Department of Pharmacy, MJP Rohilkhand University, Bareilly, UP, 243006
Akabushan@gmail.com

ABSTRACT

Green synthesis has gained attention as a cleaner, more sustainable way to produce nanoparticles, using plant phytochemicals in place of the harsh chemical reducing agents traditionally required. Compounds naturally present in plants, such as polyphenols and flavonoids, can reduce metal precursors while also capping and stabilizing the resulting nanoparticles, removing the need for hazardous reagents altogether. When phytoconstituents are incorporated into these nanocarriers, several long-standing problems with plant-based medicines, namely poor solubility, weak stability, and low bioavailability, can be significantly improved. The resulting nanophytomedicines have shown notable antioxidant, anti-inflammatory, antimicrobial, anticancer, and immunomodulatory activity, largely because nanoscale formulation improves cellular uptake and allows more efficient interaction with biological targets, including modulation of oxidative stress, suppression of inflammatory cytokines, and activation of apoptotic pathways in cancer cells. Progress in surface engineering has also made it possible to design nanophytomedicines that respond to specific physiological triggers, allowing more targeted delivery and reducing unwanted effects on healthy tissue. Even so, several obstacles still stand in the way of clinical use. The underlying mechanisms of action are not yet fully understood, synthesis methods vary widely between studies, long-term safety data are limited, and reliable large-scale production remains difficult to achieve. Moving forward, research needs to focus on clarifying these mechanisms, conducting thorough safety evaluations, standardizing synthesis procedures, and developing scalable production methods, steps that will be essential if nanophytomedicines are to move from the laboratory into real clinical practice.

Natural Oils as Complementary Therapies for Holistic Management of Psoriasis and Vitiligo

Priyanshi Priya, Ishu Garg
College of Pharmacy, Shivalikh Campus, Shivalikh University, Sherpur, Dehradun-248197, Uttarakhand, India
priyanshipriya9570@gmail.com

ABSTRACT

Psoriasis and vitiligo are chronic autoimmune skin disorders characterized by dysregulated immune responses and persistent inflammation. Although conventional treatments such as corticosteroids and immunomodulators remain standard, their prolonged use is often limited by side effects and high relapse rates. Natural oils rich in essential fatty acids, antioxidants, and bioactive compounds have demonstrated anti-inflammatory, antioxidant, and immunomodulatory properties. These agents not only improve skin hydration but also modulate keratinocyte proliferation, melanocyte function, and immune signaling. Certain oils have demonstrated dual efficacy in psoriasis and vitiligo models, suggesting broader dermatological applications. However, inconsistent outcomes across studies are attributed to variability in oil composition, extraction processes, and application protocols. Natural oils represent promising complementary therapies for psoriasis and vitiligo. Nonetheless, standardized formulations, dose optimization, and robust clinical trials are necessary to validate their efficacy and ensure reproducible outcomes in dermatological care.

Keywords: Psoriasis, Vitiligo, Natural Oil, Anti-inflammatory, Immuno-modulatory, Anti-oxidant, Natural therapy

Type II Diabetes Mellitus Management Clinical Complications and the Expanding Role of Nutraceuticals, Phytotherapeutics, and Novel Therapies

Parineeti Priya, Ishu Garg

College of Pharmacy, Shivalikh Campus, Shivalikh University, Sherpur, Dehradun-248197, Uttarakhand, India

parineetipriya9570@gmail.com

ABSTRACT

Diabetes mellitus (DM) has a complex etiology and is a long-term, multifaceted metabolic disease resulting from anomalies in insulin secretion, insulin action, or both. The global burden of DM continues to rise, accompanied by severe microvascular and macrovascular complications that significantly impact quality of life and healthcare systems. Diabetes management involves conventional therapeutic strategies lifestyle modification, synthetic oral antihyperglycemic agents, nutraceuticals, phytotherapeutics, insulin therapy, and digital health interventions. In clinical practice, the combined use of oral antidiabetic drugs, insulin, nutraceuticals, and phytotherapeutics is common; however, such combinations may result in beneficial or adverse interactions, highlighting the need for precise and evidence-based evaluation. Emerging and advanced therapeutic approaches, such as stem cell therapy, gene and mRNA-based interventions, artificial pancreas systems, and bioelectronic devices, are the future of diabetic management, with some already translated into clinical use. The integrative review emphasizes the importance of combining conventional treatments with evidence-based nutraceutical, phytotherapeutic, and technological innovations for improved diabetes management.

Keywords: Anti-diabetic agents, Artificial pancreas, Bioelectronics, Insulin, Nanotechnology, Nutraceuticals, Phytotherapeutics

Formulation & Evaluation of (Chalcone Based- Semi Synthetic) *Nano-Gel* for their, Enhanced Anti-Inflammatory & Analgesic activities

Pathan Muzakkir Ahmed Nisar Ahmed*
Dept. of Pharmaceutics, RP College of Pharmacy, Dharashiv, MH, 413501
Dept. of Pharmaceutical Chemistry, RP College of Pharmacy, Dharashiv, MH, 413501.
p.muzakkir99@gmail.com

ABSTRACT

Chalcones are a class of natural compounds that exhibit promising anti-inflammatory and analgesic properties, exemplified by compounds such as Curcuminoid chalcone and Naringenin chalcone. However, their therapeutic potential is often hindered by poor solubility and bioavailability. While various formulations are available, there is a pressing need to develop semi-synthetic Nano-formulations that can provide rapid effects with minimal side effects. The primary purpose of this work is to design and obtain a series of Chalcone-based semi-synthetic Nano-Gels, specifically the Chalcone–NSAID Herbal formulation. This formulation aims to target arthritis, gout, tendinitis, and inflammation—conditions that significantly affect many elderly individuals. By combining chalcones with herbal components, the formulation seeks to leverage the synergistic effects of both, enhancing therapeutic benefits. Chalcones are recognized for their anti-inflammatory and analgesic properties, while the addition of herbs can contribute additional therapeutic benefits, optimizing treatment outcomes. The development of a Nano formulation that uniquely combines chalcones with herbal components aims to enhance the treatment of inflammation and analgesia. By utilizing nanotechnology, this formulation seeks to improve the solubility and bioavailability of chalcones and herbal medicine, allowing for more effective therapeutic outcomes. This innovative approach offers a promising strategy for optimizing treatment while minimizing side effects.

Keywords: Chalcone, Nano-gel, Anti-inflammatory, Analgesic, Semi-synthetic.

Applications of Carbon Nanotubes in Bone Targeting Functionalization Strategies, Therapeutic Platforms and Translational Barriers

Rinku Y. Patil[1], Akshada A. Koparde[2], Sujata A. Jadhav[3]

*1 PhD Research Scholar, Department of Pharmaceutical Sciences, Krishna Institute of Pharmacy, Krishna Vishwa Vidyapeeth (Deemed to be University), Karad, Maharashtra, India *rinkujadhav742@gmail.com*

2 Associate Professor & Dean Academics, Department of Pharmaceutical Chemistry, Krishna Institute of Pharmacy, Krishna Vishwa Vidyapeeth (Deemed to be University), Karad, Maharashtra, India

3 Professor, Department of Pharmacology, Krishna Institute of Medical Sciences, Krishna Vishwa Vidyapeeth (Deemed to be University), Karad, Maharashtra, India

rinkujadhav742@gmail.com

ABSTRACT

Bone diseases including osteoporosis, osteosarcoma, bone metastases and non-union fractures require drug delivery to a dense, poorly perfused mineralised compartment that systemic agents reach inefficiently. Dose escalation to compensate produces off-target toxicity. Carbon nanotubes offer high aspect ratio, high surface area, mechanical strength and tuneable surface chemistry, making them promising carriers for bone-targeted therapy. Literature published between 2015 and 2025 was searched in PubMed, Scopus and Web of Science using terms combining carbon nanotube descriptors with bone targeting, hydroxyapatite affinity and osteotropic delivery. Studies reporting functionalization chemistry, targeting ligand selection or biological evaluation were included. Bone selectivity is engineered rather than intrinsic, conferred by conjugating mineral-binding ligands to carboxyl groups introduced at oxidised nanotube tips and sidewall defects, most commonly via EDC/NHS coupling. Reported ligands include bisphosphonates (alendronate, risedronate, zoledronate) and oligo (aspartic acid) sequences, both binding hydroxyapatite through calcium chelation. Single-walled nanotubes predominate in imaging and sensing applications, multi-walled nanotubes in scaffold reinforcement and high-payload delivery. Documented functions span chemotherapeutic and nucleic acid delivery, near-infrared photothermal ablation, photoacoustic and Raman imaging, and biomarker sensing. Limitations include incompletely characterised long-term toxicity, unstandardised synthesis and functionalization, poorly defined clearance pathways, and absent CNT-specific regulatory guidance. Functionalized carbon nanotubes combine mineral-binding selectivity with high payload capacity and multimodal function in a single platform. In the reviewed literature, evidence frequently relies on cell-free hydroxyapatite binding assays as a primary demonstration of bone selectivity. Mineral affinity is necessary for bone targeting but not sufficient to establish accumulation or therapeutic benefit.

Keywords: carbon nanotubes; bone targeting; hydroxyapatite affinity; bisphosphonate functionalization; nanotheranostics; targeted drug delivery.

Long-Acting MethylcobalaminFormulations a Comprehensive Review of Photodegradation Mechanisms, Encapsulation Challenges, and Emerging Sustained-Release Strategies

Aryan Gupta[a], Vivek Srivastava[a]*
[a] *Department of Pharmaceutical, school of pharmacy, Parul University, Gujarat, India*
vivek.shrivastava121147@paruluniversity.ac.in

ABSTRACT

Methylcobalamin (MeCbl), an active coenzyme form of vitamin B12, is widely used in the management of vitamin B12 deficiency and neurological disorders. However, its development as a long-acting formulation is challenging because of its high aqueous solubility, rapid clearance, pronounced photodegradation, and susceptibility to oxidative degradation. These limitations can affect drug stability, encapsulation efficiency and duration of therapeutic action. This review critically examines approaches for improving the stability and sustained delivery of methylcobalamin. Particular emphasis is given to the mechanisms of photodegradation and the influence of formulation and environmental factors. Various delivery platforms, including PLGA and PLA microparticles, nanoparticles, liposomes, cyclodextrin inclusion complexes, hydrogels and injectable depot systems, are evaluated with respect to encapsulation efficiency, photoprotection and release characteristics. Important preparation techniques, including the W/O/W double-emulsion method, and analytical approaches such as RP-HPLC and LC-MS/MS are also discussed. The review indicates that biodegradable polymeric systems, particularly PLGA-based microparticles, offer considerable potential for sustained methylcobalamin delivery. However, the hydrophilic nature of methylcobalamin may result in low encapsulation efficiency and initial burst release. Cyclodextrin complexation can provide enhanced photoprotection but has limited sustained-release capability when used alone. Therefore, combining photoprotective strategies with biodegradable polymeric carriers represents a promising approach for developing long-acting formulations. Long-acting methylcobalamin formulations may overcome major limitations associated with photodegradation, high aqueous solubility and repeated administration. PLGA-based depot systems combined with suitable photoprotective strategies such as cyclodextrin complexation appear particularly promising. Further research is required to optimize formulation parameters, improve scalability, and establish long-term safety and efficacy.

Keywords: Methylcobalamin; Vitamin B12; Sustained-release; Photodegradation; PLGA; Drug delivery; Encapsulation; Controlled release.

Optimization of Monoterpene-Loaded Transferosomes for Enhanced Transdermal Delivery in Rheumatoid Arthritis Treatment

Harsh Rastogi[1], Manu Sharma[2]
[1]*Research Scholar, Department of Pharmacy, Banasthali Vidyapith, Jaipur, Rajasthan, India*
[2]*Associate Professor, Department of Pharmacy, Banasthali Vidyapith, Jaipur, Rajasthan, India*
* *phdprogress2025@gmail.com*

ABSTRACT

Rheumatoid arthritis (RA) is a chronic inflammatory autoimmune disorder requiring prolonged pharmacotherapy, often associated with frequent dosing and systemic adverse effects. The present investigation aimed to formulate and optimize a monoterpene-loaded transfersomal gel to enhance transdermal drug delivery, improve local drug retention, and minimize systemic exposure. Monoterpene-loaded transferosomes were prepared using the lipid thin-film hydration technique. Critical formulation variables, including phospholipid concentration and cholesterol ratio, were optimized using a D-optimal experimental design. The optimized vesicular dispersion was incorporated into a Carbopol 934 gel and evaluated for physicochemical characteristics, dermal safety, skin deposition, dermatokinetic behavior, and therapeutic efficacy in an experimental rheumatoid arthritis rat model. The optimized formulation exhibited desirable vesicle characteristics with efficient skin permeation and significantly greater drug deposition within the skin compared with conventional formulations. Dermal toxicity studies confirmed good skin compatibility. In vivo evaluation demonstrated a marked reduction in paw edema following 14 days of topical treatment, indicating improved anti-inflammatory activity and enhanced localized drug delivery. The optimized monoterpene-loaded transfersomal gel offers a promising transdermal therapeutic strategy for rheumatoid arthritis by enhancing localized drug delivery, improving therapeutic efficacy, and reducing the likelihood of systemic adverse effects. These findings support its potential as an effective topical nanocarrier system for long-term RA management.

Keywords: Monoterpene-loaded transferosomes; Transdermal drug delivery; Rheumatoid arthritis; D-optimal design; Transfersomal gel.

AI-Based Evaluation of Cosmetic Formulation Ingredients for Toxicological Assessment Using Pharmacokinetics, Spectroscopic and Chromatographic Techniques

Anushree Aggarwal[1], Monika Bhardwaj*
KIET School of Pharmacy, KIET Deemed to be University, Ghaziabad, India
monika.bhardwaj@kiet.edu

ABSTRACT

The safety of cosmetic products is highly important to avoid health hazards to the consumers due to the use of certain ingredients some of which may exhibit noxious, mutagenic or carcinogenic effects. Identification and evaluation of such compounds are essential components of product development and quality control. Pharmacokinetic, toxicological and analytical techniques including High-Performance Liquid Chromatography (HPLC), and Gas Chromatography- Mass Spectrometry (GC-MS) are widely employed to exemplify cosmetic ingredients and perceive impurities, while Artificial Intelligence (AI) offers a complementary approach to interpreting the resulting analytical data.Cosmetic formulation ingredients were analyzed for pharmacokinetic, toxicological and chromatographic data by ADMET, HPLC and GC-MS experiments. The resulting data sets of such experiments were processed using AI-based predictive models for identification of cosmetic ingredients, detect trace impurities, and assess potential toxicity, including mutagenicity and carcinogenicity, based on structure activity relationships.AI, combined with pharmacokinetic, toxicological and chromatographic data, allowed for fast and accurate detection of cosmetic ingredients and their related impurities. Using AI-powered toxicity prediction models, they were able to identify potentially problematic compounds. This provides a faster and more accurate analysis than manual methods, while maintaining consistency across large datasets. Using AI together with advanced analytical techniques offers an efficient, modern strategy for the toxicological evaluation of cosmetic ingredients. It helps in the early identification of harmful compounds, improves quality control, and could lessen the need for animal testing while enhancing regulatory compliance and consumer safety, thus providing a valuable direction for future cosmetic safety evaluation.

Keywords: Cosmetic safety, Artificial Intelligence, Pharmacokinetics, HPLC, GC-MS, Toxicological assessment

A pH-Triggered In-Situ Gelling System for Ocular Drug Delivery

Devanshi Sharma
[1]KSOP, KIET Groups of Instituions, Uttar Pradesh, India
devanshi.2377sharma@gmail.com

ABSTRACT

Maintaining an effective drug concentration at the ocular surface is a persistent formulation challenge. Conventional eye drops are rapidly cleared by tear turnover, reflex blinking, and nasolacrimal drainage, limiting ocular bioavailability to below five percent and requiring frequent dosing. pH-triggered in-situ gelling systems address this by remaining as low viscosity, easily installable liquids at formulation pH while undergoing a rapid sol-to-gel transition on contact with the near-neutral pH of tear fluid, prolonging precorneal contact time. This review was developed by surveying peer-reviewed research articles, reviews, and patent literature on pH-responsive ocular in-situ gelling systems, focusing on polyacrylic acid (Carbopol)-based formulations. Sources were assessed for gelling polymer composition, mechanism of gelation, in-vitro/in-vivo evaluation parameters (gelation pH, viscosity, drug release, ocular tolerance), and reported therapeutic outcomes, to compile a comparative synthesis of the approach. Carbopol emerged as the principal pH-sensitive polymer in ocular in-situ gels, undergoing sol-to-gel transition through ionisation and swelling of its carboxylic acid groups as pH shifts from the acidic formulation state toward the tear-fluid pH of approximately 7.4. Its inherently acidic, potentially irritant nature was consistently offset by co-formulating with viscosity-enhancing, mucoadhesive polymers such as hydroxypropyl methylcellulose or chitosan. Formulations carrying model drugs including ciprofloxacin hydrochloride, baicalin, brimonidine tartrate, timolol maleate, and gatifloxacin showed extended precorneal retention, sustained release over six to eight hours, several-fold gains in ocular bioavailability over conventional solutions, reduced systemic absorption, and largely non-irritant profiles in corneal and chorioallantoic membrane irritation assays. Carbopol-based pH-triggered in-situ gels, especially when combined with mucoadhesive or viscosity-modifying co-polymers, offer a clinically promising, patient-compliant alternative to conventional eye drops by improving precorneal residence and bioavailability while reducing dosing frequency. Formulation-related acidity and limited clinical translation remain areas for further research.

Keywords: In-situ gel, pH-triggered, Carbopol, Ocular drug delivery, Mucoadhesion, Bioavailability

Poly-pharmacology in Modern Drug Design: Rationale, Applications, and Emerging Computational Approaches

Aayushi Aggarwal[1], Megha Garg[1*]
[1]School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
aayushiaggarwal2989@gmail.com

ABSTRACT

For a long time, conventional drug discovery has emphasized highly selective molecules aimed at a particular biological target by following the "one drug, one target" approach. However, the efficacy of single-target agents gets limited due to several interconnected pathways and biological targets, which are associated with complex diseases including cancer, diabetes and neuropsychiatric disorders. Polypharmacology attempts to overcome this complexity by finding or designing a single drug that can act on multiple relevant molecular targets at the same time. Compared with combination therapy, rational multi-target approaches may simplify treatment regimens and reduce certain drug-drug interaction risks, although achieving an optimal balance between therapeutic efficacy and off-target effects remains challenging. Several recognised drugs like clozapine, which interacts with multiple neurotransmitter receptor systems, and sunitinib, which inhibits multiple receptor tyrosine kinases associated in tumor growth and angiogenesis demonstrate clinically relevant multi-target activity. Computational tools such as network pharmacology, molecular docking and in silico target prediction platforms like SwissTargetPrediction and PharmMapper are increasingly used to explore drug target interactions and prioritise promising candidates before experimental testing begins. This review aims to discuss the rationale and therapeutic applications of polypharmacology by focusing on multi-target drugs, and explores how these computational approaches are influencing multi-target drug discovery. It also considers key challenges including target selectivity, toxicity, pharmacokinetic complexity and the need for experimental validation, while highlighting future opportunities for rational polypharmacological drug design.

Keywords: Polypharmacology, Multi-target drugs, Drug discovery, Network pharmacology, Molecular docking, Computational drug design.

3D-Printed Drug Delivery Systems: Advances in Personalized and Controlled Drug Delivery

Aditya[1], Megha Garg[1]*
[1]School of Pharmacy, Krishna Institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, India
adityagorav2005@gmail.com

ABSTRACT

Three-dimensional (3D) printing is reshaping pharmaceutical manufacturing by challenging the industry's long-standing reliance on one-size-fits-all dosing, allowing precise control over a formulation's shape, composition, drug loading, and release behavior to open the door to genuinely individualized medicine. This review explores the four leading 3D printing techniques used in drug delivery: fused deposition modeling, stereolithography, selective laser sintering, and semi-solid extrusion, examining how each process works, its particular strengths, and the ways it's currently being applied, with a central focus on personalized medicine applications such as patient-specific dosage forms, polypills that combine several drugs into a single dose, formulations designed around the needs of pediatric and geriatric patients, and implantable or fast-dissolving dosage forms, as well as how multi-material and multi-layer printing can be leveraged to engineer programmed, controlled drug release alongside the expanding use of biocompatible and biodegradable printing materials. That said, the field still has real obstacles to work through, including formulation optimization, printability, dose uniformity, quality control, scalability, long-term stability, and a regulatory landscape that hasn't fully kept pace with the technology, yet despite these challenges, 3D printing represents a promising path toward more flexible, personalized, and controlled drug delivery systems, with the potential to play a significant role in the future of patient-centered pharmaceutical manufacturing.

Keywords: Drug Delivery Systems, Personalized Medicine, Controlled Drug Release, Fused Deposition Modeling (FDM), Stereolithography (SLA), Polypills.

Role Of Nanomedicine in Pancreatic Cancer

Prince Singh[1], Paramvir Malik[2,], Akansha Jain[1*]
Meerut Institute of Engineering and Technology
akansha.jain@miet.ac.in

ABSTRACT

Genetic abnormalities, increased interstitial fluid pressure, and a thick tumor stroma all contribute to the complicated microenvironment of PDAC.This greatly increases the risk of metastasis and drug resistance, making it more difficult for traditional chemotherapy treatment methods to effectively deliver therapeutic drugs. Onivyde and Abraxane are the two nanoformulations that the FDA has so far approved exclusively for the treatment of PDAC. Compared to traditional gemcitabine-based treatments, Onivyde, a pegylated liposome formulation of irinotecan. When combined with gemcitabine, abraxane, a paclitaxel nanoparticle albumin-bound formulation. Short chain pegylated lipids, have been added to lipid nanoparticles (LNPs) to reduce PEG-mediated steric hindrance and improve NP-cell interaction. These shorter chains improve cellular interaction and transfection efficacy because they disappear more quickly in the circulation than their long-chain analogs. The current vaccines for SARS-CoV-2 are being tested in clinical trials show that using this approach is successful in mRNA-loaded LNPs. Faster PEG detachment might reduce the circulatory half-life and systemic stability, which might limit the NPs' total therapeutic window. The topic of nanomedicine in PDAC treatment offers a lot of room for research and development after the FDA approved Abraxane and Onivyde. Due to their very "simple" architecture, these two medications primarily depend on passive targeting methods to deliver a single drug. Further research combining these nanomedicines with tumor-penetrating peptides may yield important new information and advancements in targeting effectiveness, removing present obstacles, and boosting the efficacy of nanomedicine in PDAC treatment.

Keywords: Pancreatic ductal adenocarcinoma, chemoresistance, nanomedicine, signaling pathway

Metallic Nanoparticles as Noval Antifungal Agents

Paramvir Malik[1], Prince Singh[2], Akansha Jain[1*]
Meerut institute of engineering and technology, Baghpat road Meerut
akansha.jain@miet.ac.in[1*]

ABSTRACT

Fungal infections (FIs) cause a variety of illnesses in people, from invasive FIs that can be fatal to skin infections. There are currently about 300 fungal species known to cause different fungal illnesses in people. Effective antifungal therapy depends critically on early diagnosis and treatment. To eradicate mucormycosis, further treatments and surgical excision of all infected tissues are crucial. Nanotechnology is the study and manipulation of substances' characteristics through size control. Innovations in nanotechnology have recently surfaced as successful strategies for overcoming medication resistance. In order to effectively combat FIs and overcome fungal multi-resistance to currently available AFAs, NP-based drug delivery methods offer a promising alternative for developing fresh pharmaceutical formulations. Because pathogens are less likely to become resistant to NPs, NPs are widely utilized in nanomedicine to treat bacterial and fungal diseases. DDSs are designed in such a way that they can serve as drug reservoirs (for example, as sustained-release systems) and/or change the biodistribution and pharmacokinetics of their associated drugs. Indeed, new techniques are urgently needed to fight against resistant microorganisms in order to decrease the clinical burden. The use of MNPs, such as gold (Au), platinum (Pt), silver (Ag), zinc (Zn), iron (Fe), copper (Cu), and many more, in medicine is gaining attention. Ag, Au, and Pt are among the noble MNPs that have been used in a variety of medicinal applications, such as gene delivery and antifungal therapy. Though further work is needed to find new targets and create NP-based AFAs, the current development of novel AFAs mostly focuses on structural alteration to improve their safety and efficacy. On the other hand, the physicochemical characteristics, dosage, and mode of administration of metal nanoparticles in humans are associated with any possible risk of harmful or hazardous outcomes. Extensive physicochemical characterization is necessary in the early phases of therapies development since MNPs usually have a limited therapeutic window.

Keywords: Fungal infections, Antifungal agents, Metallic nanoparticles, gold nanoparticles, silver nanoparticles

A Comprehensive Review on Recent Advances And Patents Of Nanorobotics And Nanosensors In Healthcare

Vansh Bhargav[1*], Tannu[1], Harsh Chikara[1], Harsh Goswami[1], Sonal Sharma[1], Monika Sachdeva[1]
[1] Raj Kumar Goel Institute of Technology (Pharmacy), Raj Nagar Extension, Ghaziabad, Uttar Pradesh, India, 201017
vb638603@gmail.com

ABSTRACT

Nanorobotics and nanosensors are the two most disruptive pillars of healthcare innovation based on nanotechnology and work with dimensions on the 1-100nm scale to interface with biological systems at a molecular scale. This Comprehensive review examines in-depth more recent developments (2018-2026) and the international patent portfolio (United States (USPTO), European Union (EPO), India (IPO/CGPDTM), Japan (JPO), China (CNIPA), and PCT international patents) of nanorobotics and nanosensors used in healthcare applications. The current state of nanorobotics development includes the delivery of drugs using DNA-origami, magnetically driven surgical nanobots, biohybrid motors based on bacteria, and swarm systems controlled by AI. In breakthroughs, nanosensors have been used to achieve single-molecule detection using surface-enhanced Raman scattering (LOD ~10^{-18} M), and the detection of circulating tumour DNA and cancer biomarkers using electrochemical nanosensors, nanosensor arrays on wearable, and implantable nanosensors to monitor glucose continuously. India has also become a key player with 271 IPO filings in 2024, with a growth rate of 35-40 % per annum, mainly IIT, CSIR, IISc and most of the pharmaceutical institutions. The translational barrier between laboratory demonstration and clinical application is the most significant issue, even with outstanding scientific advancements. The most significant obstacles are biocompatibility and immunogenicity, consistent in-vivo navigation and real-time tracking, miniaturisation of power source, development of regulatory framework and scale-up of manufacturing.

Keywords: Nanorobotics; nanosensors; nanomedicine; drug delivery; targeted therapy; biosensors; magnetic nanorobots; SERS; electrochemical sensing; Indian patents; USPTO; EPO; clinical translation; precision medicine; theranostics.

Computer Aided Design Tools For Innovation in Pharmaceutical Sciences

Shafi Shah, Arjun Nagar
Sanskar College of Pharmacy and Research, Ghaziabad, U.P., India
Shafishah07866@gmail.com

ABSTRACT

Computer-aided design (CAD) tools have emerged as important technologies for promoting innovation in pharmaceutical sciences. These computational approaches assist researchers in designing, predicting, and optimizing drug molecules and pharmaceutical formulations before extensive laboratory experimentation. Computer-aided drug design (CADD) techniques such as molecular docking, virtual screening, molecular dynamics simulation, quantitative structure–activity relationship (QSAR) analysis, and pharmacophore modelling are widely used to identify potential drug candidates and predict their interactions with biological targets. These tools can help reduce the time, cost, and resources required during the early stages of drug discovery. In addition to drug discovery, computer-aided approaches are increasingly being applied in pharmaceutical formulation and drug delivery. Computational modelling can support the optimization of drug–excipient interactions, dosage forms, drug-release profiles, and delivery systems. Artificial intelligence (AI) and machine learning further enhance these capabilities by analysing large datasets and identifying patterns that may not be easily recognized through conventional methods. CAD-based approaches can therefore facilitate rational decision-making and improve the efficiency of pharmaceutical research and development. Despite their advantages, computational predictions require experimental validation, and factors such as data quality, model limitations, and computational requirements must be considered. Overall, computer-aided design represents a valuable and rapidly developing approach in pharmaceutical sciences, with considerable potential to accelerate drug discovery, optimize formulations, reduce development costs, and support the development of safer and more effective medicines.

Keywords: Computer-Aided Design, Computer-Aided Drug Design, Molecular Docking, Artificial Intelligence, Drug Discovery, Pharmaceutical Innovation.

Editing Life: The CRISPR Revolution

Anas Sayyed
Sanskar College of Pharmacy and Research, Ghaziabad
anasalisayyed556@gmail.com

ABSTRACT

CRISPR is a revolutionary gene-editing technology that uses guide RNA and the Cas9 enzyme to precisely cut and modify DNA. Unlike traditional gene-editing methods, CRISPR is direct, fast, efficient, and relatively simple, allowing researchers to delete, insert, or correct specific genes. Earlier tools such as ZFN and TALEN were generally expensive, complex, and time-consuming, which encouraged the development and wider adoption of CRISPR as a more accessible and precise approach. CRISPR was first introduced in 2014 for the treatment of Duchenne Muscular Dystrophy (DMD) in a mouse model. Following this successful experimental work, the technology attracted considerable attention in biomedical research and therapeutic applications. Currently, CRISPR is being widely studied for genetic disorders such as sickle cell anemia and cystic fibrosis, as well as for cancer gene therapy. It is also being evaluated for viral diseases such as HIV and is considered a promising approach in modern gene therapy. CRISPR has shown important progress in DMD and sickle cell anemia, while research continues for other complex disorders including cancer and HIV. Beyond medicine, CRISPR has valuable applications in agriculture for crop improvement, biotechnology research, animal science, and forensic science. Overall, CRISPR represents a major advancement in genetic engineering and has significant potential for future therapeutic and research applications.

Keywords: CRISPR, gene editing, genetic disorders, cancer therapeutics

Extracellular Vesicles as Natural Nanocarriers for Targeted Drug Delivery

Aleena Sayyed
Sanskar College of Pharmacy and Research, Ghaziabad
aleenasayyed7037@gmail.com

ABSTRACT

Extracellular vesicles (EVs) are nano-sized, lipid bilayer-enclosed particles naturally secreted by almost all cell types and play a crucial role in intercellular communication through the transfer of proteins, lipids, and nucleic acids. In recent years, EVs, particularly exosomes, have emerged as promising drug delivery vehicles due to their intrinsic biocompatibility, low immunogenicity, stability in circulation, and ability to cross biological barriers such as the blood-brain barrier. Unlike conventional synthetic nanocarriers, EVs possess inherent targeting capabilities mediated by surface adhesion molecules and membrane proteins, enabling selective delivery to recipient cells. EVs can be engineered to encapsulate a wide range of therapeutic cargo, including small-molecule drugs such as cisplatin, siRNA, miRNA, mRNA, CRISPR/Cas components, and proteins, using both endogenous loading strategies (cell engineering) and exogenous methods (electroporation, sonication, and incubation). Preclinical studies have demonstrated their therapeutic potential in cancer, neurodegenerative disorders, cardiovascular diseases, and inflammatory conditions. However, challenges remain in large-scale production, purification standardization, cargo loading efficiency, and safety profiling. Overall, extracellular vesicle-based drug delivery systems represent a rapidly advancing frontier in nanomedicine, offering a biologically inspired platform for targeted and personalized therapeutics. Continued optimization of engineering strategies and manufacturing processes will be critical for successful clinical translation.

Keywords: Extracellular vesicles, Exosomes, Drug delivery, Nanocarriers, Targeted therapy

Extracellular Vesicles as Natural Nanocarriers for Targeted Drug Delivery

Ikra
Sanskar College of Pharmacy and Research, Ghaziabad
rukhsarsaifi905@gmail.com

ABSTRACT

Extracellular vesicles (EVs) are nanoscale, lipid bilayer-enclosed particles that are naturally released by nearly all cell types and have an important role in cell-to-cell communication by transporting proteins, lipids, and nucleic acids. In recent years, EVs, especially exosomes, have gained considerable attention as promising drug delivery carriers because of their natural biocompatibility, low immunogenicity, stability within the circulation, and capacity to pass biological barriers, including the blood-brain barrier. In contrast to conventional synthetic nanocarriers, EVs have intrinsic targeting properties that are mediated by membrane proteins and surface adhesion molecules, allowing selective transport of therapeutic substances to recipient cells. EVs can be designed to carry a broad variety of therapeutic cargos, such as small-molecule drugs including cisplatin, siRNA, miRNA, mRNA, CRISPR/Cas components, and proteins, through endogenous loading approaches (cell engineering) as well as exogenous techniques (electroporation, sonication, and incubation). Preclinical research has shown their therapeutic promise in cancer, neurodegenerative diseases, cardiovascular disorders, and inflammatory conditions. Nevertheless, important limitations include large-scale manufacturing, standardized purification, efficient cargo loading, and comprehensive safety evaluation. Overall, EV-based drug delivery systems constitute a rapidly developing area of nanomedicine and provide a biologically inspired approach for targeted and personalized therapy. Further improvement of engineering methods and manufacturing procedures will be essential to enable successful clinical translation.

Keywords: Extracellular vesicles, Exosomes, Drug delivery, Nanocarriers, Targeted therapy

Computer Aided Design Tools for Innovation In Pharmaceutical Sciences

Annu Yadav*, Harsh Chauhan
Sanskar College of Pharmacy and Research, Ghaziabad, U.P, India
Yadavansh4733@gmail.com

ABSTRACT

The pharmaceutical industry is undergoing a major technological transformation in which computer-aided design (CAD) tools are becoming increasingly important for developing new therapeutic agents and pharmaceutical products. These tools combine computational chemistry, mathematical modelling, data analysis, and simulation to support rational decision-making throughout the drug-development process. In early drug discovery, techniques such as de novo drug design, molecular docking, virtual screening, pharmacophore modelling, and quantitative structure–activity relationship (QSAR) studies allow researchers to explore large chemical spaces and select promising molecules for further investigation. In silico prediction of absorption, distribution, metabolism, excretion, and toxicity (ADMET) can further assist in identifying candidates with favourable drug-like characteristics before extensive experimental testing. The combination of CAD with artificial intelligence and machine-learning algorithms offers additional opportunities for recognizing complex patterns, generating novel molecular structures, and optimizing pharmaceutical systems using available experimental data. These approaches can reduce repetitive laboratory experiments and enable researchers to focus resources on the most promising candidates. However, the reliability of computational predictions depends considerably on the quality of input data, appropriate model selection, and experimental validation. Computer-aided design tools therefore serve not as replacements for laboratory research but as powerful complementary technologies capable of promoting faster, economical, and scientifically guided innovation in pharmaceutical sciences.

Keywords: Computer-aided design, CADD, in silico methods, ADMET, molecular modelling, pharmaceutical formulation, nanomedicine, artificial intelligence.

Role of Bioinformatics in Modern Pharmaceutical Research

Shivani yadav, khushboo Bansal
Department of pharmaceutics, Sunderdeep Pharmacy Collage, Dasna, U.P, India
Shivaniyadavasan@gmail.com

ABSTRACT

Bioinformatics is an interdisciplinary field that integrates biology, computer science, and information technology to analyze complex biological data. It has become an important tool in modern pharmaceutical research for drug–target identification, disease analysis, and drug discovery. Bioinformatics approaches include genomic and proteomic analysis, sequence analysis, protein structure prediction, molecular docking, virtual screening, pharmacophore modeling, and molecular dynamics studies. These computational techniques help researchers investigate drug–target interactions and predict important properties of potential drug candidates. The application of bioinformatics enables rapid screening of large numbers of molecules and identification of promising therapeutic candidates. Integration with artificial intelligence and machine learning can further improve prediction of biological activity, drug interactions, pharmacokinetic properties, and toxicity. Bioinformatics provides efficient and cost-effective approaches for modern pharmaceutical research. Its integration with computer-aided drug design and artificial intelligence can accelerate drug discovery and improve candidate selection. However, computational findings require experimental validation before clinical application.

Keywords: Bioinformatics; Drug Discovery; Molecular Docking; Virtual Screening; Drug Targets; Artificial Intelligence; CADD.

Explainable AI-Driven CADD: making AI-Powered Drug Discovery Transparent, interpretable and Trustworthy

Kritika, Khushboo Bansal*
Sunderdeep Pharmacy College, SDGI Global University, Dasna, Uttar Pradesh, India
0609kritika@gmail.com

ABSTRACT

Predictions of chemical characteristics, target interactions, affinity, toxicity, and pharmacokinetics are accelerated by AI-driven CADD; nonetheless, deep-learning models continue to be opaque "black boxes." In order to address this, XAI explains how and why these algorithms generate their forecasts. In order to increase the transparency and dependability of computational drug discovery, this work examines XAI within AI-driven CADD to enhance transparency and reliability in computational drug discovery. XAI techniques are applied across virtual screening, docking, ADMET prediction, repurposing, and lead identification to interpret ML predictions, identifying key descriptors, functional groups, and biological features driving activity, toxicity, and pharmacokinetics. XAI molecular modeling integration is also explored. By pinpointing the molecular and biological characteristics behind particular predictions, XAI enhances the interpretability of AI-based CADD models. This improves decision-making in ADMET evaluation, lead identification, virtual screening, and drug repurposing by boosting trust in computational results and allowing researchers and medicinal chemists to critically assess AI generated outputs. However, there are still issues, such as the complexity of the model, the low quality and limited representativeness of training data, the variety of XAI methodologies now in use, the limitations of experimentally confirming explanations, and the absence of standardized evaluation frameworks for evaluating them. A crucial step toward transparent, trustworthy, science-based drug discovery is explainable AI driven CADD. The reliability of AI-assisted judgments is strengthened when interpretability and prediction accuracy are combined, making safer and more effective treatments possible. The transparency, validity, and efficacy of computational drug development may be significantly improved by future integration with generative AI, molecular dynamics, quantum computing, multimodal biological data, and human-centered design.

Keywords: Explainable Artificial Intelligence, Computer-Aided Drug Design, Drug Discovery, Machine Learning, Molecular Modeling, ADMET, Interpretability, Trustworthy AI.

Artificial intelligence in drug discovery: From molecule to medicine

Alex Iqbal, Khushboo Bansal*
Department of Pharmaceutics, Sunderdeep Pharmacy College, Dasna, Uttar Pradesh, India
alexiqbal06@gmail.com

ABSTRACT

Drug discovery is a long, costly, and challenging process. It often takes years and millions of dollars to obtain a new pharmaceutical product. Artificial Intelligence (AI) allows pharma researchers to make this process more efficient and less time-consuming. AI-enabled technologies can analyze vast amounts of biological and chemical data to help researchers find active pharmaceutical ingredients faster by increasing speed, accuracy and efficiency of the research. The current research is based on the collective analysis of academic and scholarly articles, reports, and books that are directly dealing with the application of advanced artificial intelligence systems in drug discovery. Particular attention is paid to the methods of AI utilization in different stages and areas of drug discovery, including the preliminary discovery of drug targets, virtual screening, lead optimization, toxicity prediction, and clinical trials. The analysis revealed that AI is a disruptive technology that can radically change and improve the existing approaches to pharmaceutical drug discovery and development. AI is reported to allow discovering potential drug molecules faster than the traditional methods. Furthermore, utilizing AI can make the pharmaceutical industry more cost-effective and less wasteful. Several pharmaceutical products discovered with the help of AI are now in clinical trials. AI can reduce the time needed for drug discovery while also significantly reducing the costs of the R&D process. Thus, AI-based technologies will soon disrupt the pharmaceutical industry, opening new horizons in personalized medicine.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Pharmaceutical Research, Drug Development, Virtual Screening, Personalized Medicine.

A Systematic Review of Computational Tools Bridging in Silico Predictions and Clinical Applications of Ibuprofen

Mahak Sharma*, Bhawana Patra, Kartik Hudda, Satendra Kumar
SRM Modinagar College of Pharmacy, Faculty of Medicine & Health Sciences, SRM Institute of Science and Technology, NCR Campus, Delhi-NCR Campus, Delhi Meerut Road, Modinagar, Ghaziabad, UP, 201204, India.
mahakmadhu3@gmail.com

ABSTRACT

Ibuprofen, a commonly used non-steroidal anti-inflammatory drug (NSAID) but also an ideal compound to study the translation of computational methods. systematic assessment of the in-silico tools used to evaluate its pharmacodynamics, pharmacokinetics and toxicology. This review systematically evaluates the in-silico terrain linking molecular properties of Ibuprofen to its pharmacodynamic actions and clinical effects. A systematic literature search of the Keywords Ibuprofen, Molecular Docking, Molecular Dynamics or QSAR (quantitative structure-activity relationship), ADMET for relevant records across major databases; these are PubMed, Scopus and Web of Science.The review highlights a broad range of computational strategies used for Ibuprofen. Molecular docking studies and molecular dynamics simulations within the SBDD framework have played a key role in clarifying Ibuprofen's binding affinities against COX-1 and COX-2 enzymes, along with investigating possible off-targets interactions. Ligand-Based approaches and QSAR modeling have successfully correlated structure-activity relationships (SAR) in order to enhance efficacy and diminish gastric toxicity. Furthermore, the advanced ADMET prediction tools are being more frequently used to predict metabolism and drug-drug interactions, relating with clinical observations. This review highlights the growing use of AI and machine learning to repurpose Ibuprofen for new therapeutic indications across various diseases. This review highlights the importance of alignment of in silico protocols with experimental parameters and incorporation of AI-based predictive models that need to further expedite the clinical translation of ibuprofen along with structurally related NSAIDs.

Keywords: Ibuprofen, In Silico, Molecular Docking, ADMET, QSAR, Clinical Translation CADD.

Digital Twins in Pharmaceutical Manufacturing

Abhay Arya, Khushboo Bansal*
Department of Pharmaceutics, Sunderdeep Pharmacy College, Dasna, Uttar Pradesh, India
abhayarya7002@gmail.com

ABSTRACT

Mass production of medicines has become increasingly sophisticated, thus calling for innovative computer technologies to optimize and facilitate the manufacturing process. The adoption of Digital Twins in the pharmaceutical industry enables the creation of a virtual setting to simulate a factory model, allowing engineers to identify the most optimal parameters of operation on a digital interface prior to large-scale, capital-intensive experimentation. Through the application of real-time information exchange, engineers can construct a virtual replication of the production line to observe and optimize the manufacturing workflow. Such a twin-based concept relies on extensive data processing to forecast potential mechanical failures and examine the dynamic characteristics of the machinery, including fluid mechanics and thermal dynamics, for enhanced performance. In addition, the combination of twin technologies and artificial intelligence contributes to predictive maintenance and intelligent manufacturing that enable engineers to anticipate potential machine malfunctions. Predictive algorithms can effectively estimate pharmaceutical production outcomes, including therapeutic efficacy, chemical yields, sensor errors, and unplanned production shutdowns, during the early stages of manufacturing. Consequently, digital twin technologies integrated with real-time data exchange, advanced analytics, artificial intelligence, and predictive maintenance present a viable solution to enhance modern pharmaceutical production. The twin-based approach essentially eliminates the trial-and-error capital-intensiveness of conventional manufacturing, thereby streamlining and expediting the development and production of life-saving drug compounds.

Keywords: Digital Twins; Pharmaceutical Manufacturing; Real-Time Data; Advanced Analytics; Artificial Intelligence; Predictive Maintenance; Factory Optimization; Industry 4.0.

Role of computers in drug discovery

Aman, Khushboo Bansal*
Department of Pharmaceutics, Sunderdeep Pharmacy College, Dasna, Uttar Pradesh, India
Amanfreaktich@gmail.com

ABSTRACT

The importance of computers in research is continuously growing, especially in pharmaceutical drug formation. Previously the discover and development of drugs was primarily laboratory orientated where time and resource consumptions were tremendously high. Nowadays computers have simplified drug research work that include data analysis, molecular design, drug properties and various stages of drugs development, making its application ever since increasing time, accuracy and productivity in the pharmaceutical industry. In this study, review of relevant science articles, books and researches are examined to recognize and study the computer's utilization in drug formation and formation research, through gathering and compiling a myriad of computer-based tools and technology for drug formulation design, research on properties and development, information analysis, modeling of molecules, and even its quality testing and assurance. Information on each specific element has been gathered in the aim to examine and evaluate the computer's contribution to pharmaceutical study. Examination shows that computer has a vast and crucial contribution to all processes of the development of drug. Computer aided design has greatly assisted the researchers to discover and optimize drug molecule without consuming high quantity of time. In the field of drug designing and formulation, computational modeling of molecules offers an estimate that enable researchers and scientist to have initial indication of a drugs characteristic and effectiveness even before experimental works. Computer aids have surely contributed positively in every aspect of drugs development such as its formulation research design, properties, development, testing, quality control and quality assurance for the pharmaceutical sector of studies and industry. Therefore, with the emergence of sophisticated technologies, the use of the computer in further drug formation and study and develop will ever increase.

Keywords: Computer, Drugs Formation, CADD (Computer-Aided-Drug-Design), Modeling of Molecule, Pharmaceutical Research and Drugs Development, Quality Control, Quality Assurance.

Autism Spectrum Disorder: Pathogenesis, Biomarkers, and Therapeutic Perspectives A Review of Pharmacological and Non-Pharmacological Interventions

Ritu Raj Kumar, Dr. Sagarika Majhi*
Department of Pharmacology, I.T.S. College of Pharmacy, Muradnagar, Ghaziabad, Uttar Pradesh 201206, India
riturajkumar14082002@gmail.com

ABSTRACT

Autism spectrum disorder (ASD) is a neurodevelopmental condition marked by persistent challenges in social interaction, verbal and non-verbal communication, and restricted, repetitive behaviour patterns. This review advances current understanding of ASD neurodevelopment by emphasizing early behavioural screening, genetic evaluation, and identification of environmental risk factors, aiming to lower the overall burden of autism-related conditions. Considerable work remains in understanding and managing ASD clinically. Sustained awareness initiatives are essential for timely identification and management of affected children, alongside guidance on prenatal and pre-conception risk reduction, including counselling against consanguineous marriage, adequate maternal nutrition, and limiting environmental pollutant exposure. Expanding genetic screening and postnatal observation of feeding, nutrition, and eye-contact behaviour can enable timely intervention. Children with ASD frequently show selective eating patterns and heightened susceptibility to gastrointestinal complications, including diarrhoea, constipation, and irritable bowel syndrome. Gastrointestinal dysfunction is drawing growing scientific attention owing to the gut–brain axis linking microbiota composition with neurological function. Low-cost nutritional interventions may ease gastrointestinal and behavioural symptoms, motivating interest in individualized dietary regimens; further research should assess their generalizability across diverse populations, resource settings, and cultural contexts. Among emerging therapeutic avenues, dietary phytochemicals such as curcumin, resveratrol, naringenin, and sulforaphane show promise as neurotherapeutic agents through antioxidant, immunomodulatory, gut microbiota-regulating, and Nrf2-activating mechanisms. In silico approaches, including molecular docking, molecular dynamics simulations, DFT calculations, MM/GBSA binding free energy estimation, homology modeling, and network-pharmacology analyses, help predict the binding affinity and stability of these phytochemicals against ASD-relevant targets, guiding brain-targeted delivery system development for future research.

Keywords: Autism spectrum disorder (ASD); Neuroinflammation; Gastrointestinal (GI) dysfunction; Diagnostic biomarkers; Dietary phytochemicals; Bioactive components; In silico studies; Molecular dynamics; Density functional theory (DFT); Homology modeling; Structure-based virtual screening.

Organ-on-a-Chip: Revolutionizing Preclinical Drug Testing

Ananya Tiwari1*, Dr. Shalini K. Sawhney1, Gaurav Chaudhary1
[1] I.T.S. College of Pharmacy, Muradnagar, Ghaziabad, Uttar Pradesh 201206
ananyatiwari206@gmail.com

ABSTRACT

Conventional animal testing can be expensive, more time-consuming, ethically problematic, and sometimes not able to predict human response accurately. An organ-on-a-chip (OoC) is a small-scale laboratory device that integrates human cells, microfluidic channels and engineered biomaterials to reproduce physiological functions of a human organ. It is also known as a microphysiological system (MPS) or tissue chip that mimics the structural and functional properties of human organs using living human cells. OoC are designed to provide a more realistic model for evaluating the effects of drugs, chemicals, or diseases on the human body. They combine three components that are living human cells, microfluidic channels and physiological conditions. Human cells from a specific human organ, such as lung, liver, heart or intestine, are cultured inside the chip. Tiny channels enable the controlled flow of nutrients, oxygen, blood-like fluids and drugs, similar to the body's circulation. The chip replicates conditions found in the human body, such as fluid flow, mechanical forces, pressure, and breathing-like movements. The applications of OoC are disease modelling, personalized medicine, drug development, drug toxicity and efficacy testing. The advantages of OoC are the use of human cells to give more human relevant results, reduce animal testing, improve drug testing, mimic physiological conditions, reduce time and cost of drug development. The challenges of OoC are as it is complex technology, difficult to replicate all functions of a real organ and also requires specialized skills and equipment. OoC represents a promising technology that mimics human organ functions to improve drug safety and testing.

Keywords: Organ-on-a-Chip, Microfluidic channels, Human cells, Microphysiological system, Reduced animal testing, Human relevant results

Emerging Therapeutic Strategies for Drug-Induced Liver Injury (DILI): Advanced Approaches and Novel Medicines

Nikhil Arora[1], Dr. Sagarika Majhi[2]
[1]Research Scholar, ITS College of Pharmacy, Muradnagar
[2]Professor, ITS College of Pharmacy, Muradnagar
sagarikamajhi@its.edu.in

ABSTRACT

Drug-induced liver injury (DILI) is an important adverse drug reaction and a major cause of drug withdrawal from the market. Its clinical presentation ranges from mild, transient elevations of liver enzymes to severe hepatitis, acute liver failure and, in selected cases, the need for liver transplantation. Increasing polypharmacy and the use of multiple medicines create a continuing need for better prediction, early recognition and effective therapeutic strategies.This poster reviews current management of DILI and highlights emerging pharmacological, molecular and technology-based approaches that may improve hepatoprotection, early diagnosis and personalized treatment.A narrative review approach was used to summarize clinically relevant guidance and recent research on DILI mechanisms, risk factors, biomarkers and therapeutic strategies. Particular attention was given to approaches targeting oxidative stress, mitochondrial dysfunction, inflammation, immune-mediated injury and hepatocyte regeneration. Conventional management remains centered on prompt recognition and withdrawal of the suspected offending drug, assessment of disease severity and supportive care. N-acetylcysteine has an established role in acetaminophen toxicity and may be considered in selected clinical settings. Emerging strategies include antioxidant and anti-inflammatory approaches, mitochondrial protective agents, FXR-related therapies, regenerative and cell-based approaches, phytoconstituents, nanotechnology-based drug delivery, and gene- or RNA-targeted interventions. Investigational approaches such as mitochondria-targeted antioxidants and CYP2E1 inhibition illustrate the shift toward mechanism-based treatment. DILI remains a complex and sometimes unpredictable adverse drug reaction for which there is no single treatment applicable to all patients. Early recognition, withdrawal of the offending agent and supportive management remain the foundation of care. Future progress is likely to come from combining mechanism-based therapies with validated biomarkers, advanced human-relevant models and personalized medicine. Stronger clinical evidence is still required before most emerging approaches can become routine treatments.

Keywords: Drug-induced liver injury; hepatotoxicity; oxidative stress; mitochondrial dysfunction; biomarkers; hepatoprotection.

Effervescent Tablets for Gastric Acid-Related Disorders: A Review

Anurag Tiwari[1*], Aanchal Choudhary[1], Dr. Madhu Verma[2]
Department of Pharmaceutics, ITS College of Pharmacy, Uttar Pradesh, India
Anuragat011@gmail.com

ABSTRACT

Due to their prevalence and potential for serious complications, gastric acid-related disorders such Helicobacter pylori (H. pylori) infection, peptic ulcer disease (PUD), and gastroesophageal reflux disease (GERD) pose serious clinical problems. The first -line eradication therapy for its infection in the past depended on proton pump inhibitors (PPIs), which bind to the hydrogen - potassium ATPase pump irreversibly. Effervescent tablets offer a few benefits, including quick dissolving, the production of a tasty and stimulating drink, and possibly improved medication absorption. via the release of carbon dioxide. Effervescent tablets are uncoated tablets that contain carbonates or bicarbonates (sodium, potassium, or any other suitable alkali metal carbonate or bicarbonate) and acids (citric, tartaric, malic acid, or any other suitable acid or acid anhydrate) that react quickly in the presence of water by releasing carbon dioxide (CO2). Effervescent tablets are defined as those that are meant to dissolve or disperse in water prior to ingestion, according to a revised definition submitted to the US FDA.Binders, fillers, lubricants, and sweeteners are additional crucial excipients that contribute to the tablet's mechanical strength, palatability, and stability.They are extremely sensitive to moisture, thus in order to maintain product integrity, manufacture must be done in controlled environments, usually below 25°C and with low humidity and moisture-protective packaging. To create tablets with the right mechanical strength and dissolving characteristics, a variety of production techniques are used, including wet granulation, dry granulation, direct compression, and advanced granulation technologies including one-step granulation using water or organic solvents and two-step granulation, in which the acid and alkali phases are granulated separately.

Keywords: effervescent, proton pump inhibitor, carbonates, granulation

AI-Driven Drug Design and Discovery

Vansh Gupta*, Dr. Mukesh Kumar
Faculty of Pharmacy, Swami Vivekanand Subharti University, Meerut, Uttar Pradesh, India
Vanshgupta2008051@gmail.com

ABSTRACT

Artificial Intelligence (AI) is rapidly transforming the field of pharmaceutical research by enabling faster, data-driven approaches to drug design and discovery. Conventional drug discovery is a lengthy, costly, and high-risk process characterized by extensive experimental screening and high attrition rates. AI-driven approaches, including machine learning, deep learning, generative AI, molecular docking, quantitative structure–activity relationship (QSAR) modelling, virtual screening, and predictive ADMET analysis, provide new opportunities to address these challenges. AI can analyze large and complex datasets involving molecular structures, protein targets, biological assays, omics information, and clinical data to identify potential drug targets and predict drug–target interactions. Generative AI further enables the de-novo design of novel molecular structures with desired pharmacological and physicochemical properties. AI-assisted lead optimization can simultaneously improve potency, selectivity, solubility, permeability, metabolic stability, and safety profiles. In addition, AI supports drug repurposing, personalized medicine, biomarker identification, and optimization of clinical development. AI is consequently emerging as a powerful enabling technology for accelerating the journey from molecule discovery to medicine, while experimental and clinical validation remains indispensable.

Keywords: Artificial Intelligence, Machine Learning, Deep Learning, Drug Design & Discovery, Computer-Aided Drug Design.

Computer-Aided Design in Novel Drug Delivery Systems

Vaishnavi Gauri Vats*, Dr. Mukesh Kumar
Faculty of Pharmacy, Swami Vivekanand Subharti University, Meerut, Uttar Pradesh, India
Vaishnavigaurivats16@gmail.com

ABSTRACT

Computer-Aided Design (CAD) has emerged as a powerful technology for the development and optimization of **Novel Drug Delivery Systems (NDDS)**, offering a systematic approach to designing drug carriers, dosage forms, and delivery devices with improved therapeutic performance. Conventional formulation development often requires extensive experimentation, whereas CAD-based computational approaches can reduce development time, material consumption, and experimental workload by enabling virtual modeling, simulation, and optimization. CAD tools are increasingly applied in the design of **nanoparticles, liposomes, niosomes, micelles, solid lipid nanoparticles, nanostructured lipid carriers, hydrogels, transdermal systems, implants, and 3D-printed drug delivery systems.** Computational modeling can assist in predicting critical formulation parameters such as particle size, drug loading, encapsulation efficiency, drug release, stability, and interactions between drugs and carrier materials. Furthermore, integration of **artificial intelligence (AI), machine learning, molecular modeling, and Quality by Design (QbD)** approaches enables the identification of optimized formulations and prediction of their performance before laboratory preparation. CAD also facilitates the development of personalized and site-specific drug delivery systems, including patient-specific 3D-printed dosage forms. Despite these advantages, challenges related to model validation, data quality, computational complexity, regulatory acceptance, and translation from virtual predictions to experimental performance remain. Overall, the integration of CAD with computational modeling and AI provides a promising platform for accelerating the rational development of safer, more efficient, targeted, and personalized novel drug delivery systems.

Keywords: Computer-Aided Design, Novel Drug Delivery Systems, Artificial Intelligence, Machine Learning, 3D Printing, Quality by Design, Personalized Medicine.

Title-Development of nano emulsion system of selected oil for anti-hyperlipidemic and drug delivery of Ticagrelor

Ragini Mishra
Dr KNMIPER
rm214049@gmail.com

ABSTRACT

Hyperliedemia is a major risk factor for cardiovascular disorder and is commonly associated with poor bioavlabilty of orally administrated drug due to low solubilty. The present study focouses on the development of nano emulsion system using selected oil to enhance the anti-hyperlipdemic and drug delivery of ticagrelor. Nanoemulsion were formulated using oil, surfactant, and co-surfactant. The developed nano emulsion system has the potential to improve oral bioavlibilty and therapeutic efficacy of Ticagrelor.

Keywords: nanoemulsion; Ticagrelor; Anti-hyperlipdemic activity; Drug delivery system; Cardiovascular.

Nutraceuticals: An Emerging Branch of Pharmaceutical Science — Bioavailability and Formulation

Badal Govind Rao
Signa College of Pharmacy, AKTU
badalthakur2007@gmail.com

ABSTRACT

Nutraceuticals represent a rapidly growing intersection between food science and conventional medicine, providing physiological benefits to mitigate chronic lifestyle-driven diseases. Despite their recognized therapeutic potential, natural bioactive molecules frequently suffer from poor water solubility, chemical instability, and low oral bioavailability, which restrict their widespread clinical application. This study evaluates modern pharmaceutical formulation techniques applied to bioactive compounds. High-pressure homogenization, lipid-based nanoparticles, and liposomal encapsulation systems were designed to load model natural bioactives. The formulations were evaluated for entrapment efficiency, physical stability, in vitro drug release using simulated digestive fluids, and permeability across intestinal epithelial cell models. The optimized lipid nanoparticles demonstrated a narrow size distribution of 150–180 nm and maintained an entrapment efficiency above 85%. In vitro gastrointestinal digestion assays confirmed that encapsulation protected active ingredients from acidic degradation in the stomach. Intestinal permeability assays showed a 3.2-fold increase in bioactive transport compared with unformulated raw extracts. Utilizing advanced pharmaceutical drug delivery systems significantly improves the stability and absorption of nutraceutical compounds. Transitioning from raw natural extracts to novel nanocarriers establishes nutraceuticals as a scientifically backed, scalable discipline within mainstream pharmaceutical research and preventive healthcare.

Keywords: Nutraceuticals, Drug Delivery, Bioavailability, Lipid Nanoparticles, Preventive Healthcare

Artificial Intelligence in Drug Discovery

Riya Chaudhary[1], Ms. Bharti Chauhan[2]
[1] ITS College of Pharmacy, Ghaziabad, Uttar Pradesh, India
bhartichauhan@its.edu.in

ABSTRACT

Artificial intelligence (AI) is transforming drug discovery by making the process faster, more accurate, and cost-effective. Conventional drug discovery often takes 10–15 years and requires extensive experimental screening, resulting in high costs and a low success rate. AI integrates machine learning, deep learning, and large biomedical datasets to accelerate every stage of drug discovery, from target identification and target validation to lead identification and lead optimization. AI-powered tools can analyze complex biological data, predict protein structures, perform virtual screening of millions of compounds, and optimize lead molecules with improved efficacy and reduced toxicity. Successful examples, including INS018_055 for idiopathic pulmonary fibrosis and DSP-1181 for obsessive-compulsive disorder, demonstrate AI's potential to significantly shorten development timelines. Despite these advances, challenges such as limited data quality, lack of interpretability, biological complexity, regulatory concerns, and the need for experimental validation remain major barriers to widespread adoption. Future developments in generative AI, autonomous laboratories, digital twins, and personalized medicine are expected to further revolutionize pharmaceutical research. This presentation highlights the complete AI-driven drug discovery workflow, discusses real-world case studies, examines current limitations, and explores future opportunities. AI is not replacing scientists; instead, it is empowering researchers to make faster, data-driven decisions that can improve the efficiency of drug development and ultimately accelerate the delivery of safer and more effective medicines to patients worldwide.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning, Target Identification, Lead Optimization, Precision Medicine, Drug Development.

From Cellular Messengers to Smart Drug Carriers: Exosomes as a Next-Generation Platform for Targeted Therapy

Pushkar Sharma[1], Saloni Chauhan, Rishab Jain, Ms. Bharti Chauhan[2]
[1] ITS College of Pharmacy, Ghaziabad, Uttar Pradesh, India
pushkarsharma2200@gmail.com

ABSTRACT

Exosomes are naturally derived extracellular vesicles that have emerged as a promising next-generation platform for targeted drug delivery. They transport drugs, proteins, and nucleic acids while offering excellent biocompatibility, stability, tissue penetration, and natural cell-targeting ability. Their role in cell-to-cell communication makes them effective carriers for precision medicine. Recent advances in exosome engineering have improved drug loading, surface modification, controlled release, and selective delivery to diseased cells. Engineered exosomes carrying anticancer drugs and small interfering RNA have shown enhanced cellular uptake, reduced drug dosage, tumor suppression, and the potential to overcome drug resistance in preclinical studies. Despite these advantages, clinical translation remains challenging due to low loading efficiency, complex isolation and purification methods, batch-to-batch variation, stability issues, and difficulties in large-scale standardized production. These limitations must be addressed before widespread therapeutic use. Future research should focus on improving targeting efficiency, manufacturing consistency, safety, and long-term stability. Overall, engineered exosomes represent a highly promising strategy for developing precise, efficient, and personalized drug delivery systems for the treatment of various diseases.

Keywords: Exosomes, Drug Delivery, Targeted Therapy, Extracellular Vesicles, Cancer Therapy, RNA Interference, Precision Medicine