



**MANIPAL COLLEGE
OF PHARMACEUTICAL SCIENCES**
MANIPAL
(A constituent unit of MAHE, Manipal)



MAHE 2025
YEAR OF EXCELLENCE IN
INDUSTRY-ACADEMIA
COLLABORATIONS



MANIPAL PHARMACEUTICAL CONFERENCE

August 28-30, 2025

MPCON

2025

Theme

Translating Innovation: Bridging Pharmaceutical Research and Therapeutic Outcome

Venue: Dr. TMA Pai Halls, KMC, MAHE, Manipal

Organized by
Manipal College of Pharmaceutical Sciences
Manipal Academy of Higher Education, Manipal, India.



CONFERENCE PROCEEDINGS

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About the conference

The Manipal Pharmaceutical Conference 2025 brings together leading minds from academia, research, and industry to explore the evolving landscape of pharmaceutical sciences. Focused on the theme "Translating Innovation: Bridging Pharmaceutical Research and Therapeutic Outcome," the conference aims to foster dialogue on transforming ground-breaking research into real-world healthcare solutions. This platform will feature keynote sessions, expert panels, and research presentations that highlight advances in drug discovery, development, delivery, quality, and regulatory aspects of the field. It will also focus on the integration of cutting-edge technologies such as AI, precision medicine, and sustainable practices in Pharmaceutical Sciences, leading to bench-to-bedside therapeutic outcomes. Join us as we catalyze innovation, encourage collaboration, and shape the future of therapeutics for a healthier tomorrow.

Organizer

Manipal College of Pharmaceutical Sciences
Manipal Academy of Higher Education
Manipal 576104, Karnataka, India

COMMITTEE

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About the College

Manipal college of pharmaceutical sciences (MCOPS)

Among the colleges in India that offer professional pharmacy education, the Manipal College of Pharmaceutical Sciences - MCOPS as it is widely known as a unique standing. It is presently one of the premier institutions of the Manipal Academy of Higher Education.

MCOPS of today owes its origin to the vision and enterprise of Late Dr. TMA Pai, who ushered in an era of self-financed education, an event that changed the Indian landscape of tertiary education. A college that started offering a Diploma in Pharmacy (DPharm) education in 1963, became a degree college for a Bachelor of Pharmacy (BPharm) program in 1965. Eventually, MCOPS became the first college to offer a postgraduate course (MPharm) in Karnataka in 1970 and the Doctor of Pharmacy (PharmD) program in 2008 in India.

Approval



Pharmacy Council
of India

Accreditation



NAAC: A++
with GPA 3.65



National Board of
Accreditation

Certification



International Organization
for Standardization



BY SUBJECT 2025
Manipal Academy of Higher Education-
Manipal University (MAHE)

#101-150

QS World University Rankings by subject 2025:
Pharmacy and Pharmacology



All India NIRF Rankings 2024

Ranked **8th**
among Top
Pharmacy Institutions



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Principal & Professor
Manipal College of Pharmaceutical Sciences
MAHE, Manipal

CO-CONVENER

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Vice-Principal & Professor
Manipal College of Pharmaceutical Sciences
MAHE, Manipal

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Department of Pharmaceutical Biotechnology,
MCOPS, MAHE, Manipal

Dr. Sreedhar D

Professor
Department of Pharmaceutical Regulatory Affairs
and Management, MCOPS, MAHE, Manipal

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Department of Pharmaceutical Quality Assurance

Dr. Virendra S Ligade

Associate Professor & Head
Department of Pharmaceutical Regulatory Affairs
and Management

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Print and Media

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Venue and Entertainment Committee

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Professor & Head
Department of Pharmaceutics

Hospitality and Transportation Committee

Dr. Varadaraj Bhat

Additional Professor & Head
Department of Pharmaceutical Chemistry

Sponsorship Committee

Dr. M Surulivel Rajan

Professor & Head
Department of Pharmacy Practice

Preconference Workshops

28th August 2025 (Limited seats)

- AI in Drug Discovery and Development
- Application of DoE in Pharmaceutical Development
- Analytical Applications in Drug Discovery & Drug Delivery
- Polymerase Chain Reaction and its Applications
- Research Manuscript Preparation and Journal selection



REGISTRATION FEES

			Indian Delegates		Foreign Delegates
			MAHE	Non-MAHE*	
Conference	Regular Registration (On or before 31 July 2025)	Students	₹ 1500	₹ 1770	US\$ 200
		Others	₹ 2500	₹ 2950	
	Late/Spot Registration (After 31 July 2025)	All	₹ 3000	₹ 3540	US\$ 250
Conference and Pre-conference workshop	Regular Registration (On or before 31 July 2025)	Students	₹ 2000	₹ 2360	US\$ 250
		Others	₹ 3000	₹ 3540	
	Late/Spot Registration (After 31 July 2025)	All	₹ 3500	₹ 4130	US\$ 300

* Inclusive of GST

CALL FOR ABSTRACTS

Abstract Categories

- Pharmaceutical Chemistry & Drug Discovery
- Pharmacognosy and Phytomedicine
- Pharmacology and Biotechnology
- Pharmaceutics, Drug Delivery & Biopharmaceutics
- Pharmaceutical Analysis and Quality Assurance
- Pharmacy Practice & Clinical Pharmacy
- Drug Regulatory Affairs and Pharmaceutical Management

Important Dates

Call for Abstract	15th May 2025
Abstract Submission Deadline	10th July 2025
Abstract Acceptance Notification	15th July 2025

Abstract Acceptance Notification: within 5 working days after abstract submission deadline

CONTACT US

Email: mpcon.mcops@manipal.edu

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Department of Pharmaceutical Biotechnology
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Phone: +91-9980336315

Dr. Sreedhar D

Professor
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and Management
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Submit Abstract ▶



<https://bit.ly/mpcon2025submitabstract>

Register & Pay ▶



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MPCON 2025
 Manipal Pharmaceutical
 Conference
 29th and 30th August 2025

Preconference Workshop

Thursday, 28th August 2025

- **Registration & Breakfast:** 8:30 AM -9:30 AM
Venue: MMMC Building (next to MCOPS building), First floor lounge
- **Workshop Inauguration** (Common for all streams): 9.30 AM – 10.00 AM
Venue: Professor P. Gundu Rao Conference Hall, Ground Floor, MCOPS
- Disbursement of Batches to workshop locations: 10:00 AM -10:30 AM
- Workshop session I: 10:30 AM-12:30 PM
- Lunch: 1:00 PM -2:00 PM (Venue: NIH Food court)
- Workshop session II: 2:00 PM - 4:30 PM

Stream 1: AI in Drug Discovery and Development	
Venue: Room No. 230, Department of Pharmaceutical Chemistry, MCOPS, Manipal Faculty Coordinator: Dr Suvarna G Kini (9880713601) Resource Persons: Dr Vinod Devaraj, Senior Scientist II, Schrodinger, Bangalore Dr Dileep Kumar, Department of Pharmaceutical Chemistry, MCOPS	
10:30 AM– 11:00 AM	Smart Design of Anti-Breast Cancer Agents: AI Meets SAR for Molecular Innovation
11:00 AM – 01:00 PM	Accelerating Drug Discovery through AI-Integrated Physics-Based Modeling-Part I
01.00 PM – 02.00 PM	Lunch
02:00 PM – 04:00 PM	Accelerating Drug Discovery through AI-Integrated Physics-Based Modeling-Part II Hands-on training (Participants are suggested to bring their laptops)
04:00 PM – 04:30 PM	Discussion, Feedback, Certificate distribution, Valedictory
Stream 2: Application of DoE in Pharmaceutical Development	
Venue: Room No. 27, Department of Pharmaceutics, MCOPS, Manipal Faculty Coordinator: Dr Usha Y Nayak (9449207925)	
10:30 AM – 11:00 AM	Quality by Design and Introduction to Design of Experiments
11:00 AM – 01:00 PM	DoE; Screening designs and response surface methods
01.00 PM – 02.00 PM	Lunch
02:00 PM – 04:00 PM	Hands-on training (Participants are suggested to bring their laptops)
4:00 – 4:30 PM	Discussion, Feedback, Certificate distribution, Valedictory



MPCON 2025

Manipal Pharmaceutical
Conference

29th and 30th August 2025

Stream 3: Analytical Applications in Drug Discovery & Drug Delivery

Venue: Room No. 233, Department of Pharmaceutical Quality Assurance, MCOPS, Manipal

Faculty Coordinator: Dr Muddukrishna (8660414773) and Dr. Sachin Pawar (7020268132)

Resource Persons: Dr Gurubasavaraj HM, Principal Technical Support Specialist, Waters India

Ms Dilshad Pullancheri, Principal MS Sales Development Specialist, Waters India

10.30 AM – 11.45 AM	Oral session
11.45 AM – 01.00 PM	Basic handling of the instrument, simple analytical method development on UPLC
01.00 PM – 02.00 PM	Lunch
02.00 PM – 04.30 PM	Troubleshooting, maintenance, and applications of UPLC in drug discovery and delivery
4.30 PM – 05.00 PM	Discussion, Feedback, Certificate distribution, Valedictory

Stream 4: Polymerase Chain Reaction and its Applications

Venue: Room No. 122, Department of Pharmaceutical Biotechnology, MCOPS, Manipal

Faculty Coordinator: Dr Jesil Mathew (9342405959)

10:30 AM – 11:45 AM	Oral session
11:45 AM – 01.00 PM	Practical on Primer Designing (Participants are suggested to bring their laptops)
01:00 PM – 02:00 PM	Lunch
02:00 PM – 04:00 PM	Hands-on- PCR, Agarose Gel Electrophoresis, Data Analysis, Troubleshooting
04:30 PM – 05:00 PM	Discussion, Feedback, Certificate distribution, Valedictory

Stream 5: Research Manuscript Preparation and Journal Selection

Venue: Room No. 109, Shanbhag Seminar Hall, Department of Pharmacology, MCOPS, Manipal

Faculty Coordinator: Dr Yogendra Nayak (9448154003)

10:30 AM – 11:30 AM	Manuscript Making
11:30 AM – 01.00 PM	Managing References (Participants are suggested to bring their laptops)
01:00 PM – 02:00 PM	Lunch
02:00 PM – 02:30 PM	Journal Selection Tool
02:30 PM – 03:00 PM	Use of AI in Manuscript Writing
03:30 PM – 04:30 PM	Publication Ethics
4:30 – 5:00 PM	Discussion, Feedback, Certificate distribution, Valedictory



MANIPAL PHARMACEUTICAL CONFERENCE

August 28-30, 2025

MPCON

2025

Theme

Translating Innovation: Bridging Pharmaceutical Research
and Therapeutic Outcome

PROGRAM SCHEDULE

Day 1: THURSDAY August 28, 2025 (Pre-conference Workshop)*

Venue: Manipal College of Pharmaceutical Sciences, MAHE, Manipal, India

9:30 AM – 10:00 AM	Inauguration	Chief Guest: Dr Anil K Bhat, Dean, KMC Manipal, MAHE, Manipal
Time	Preconference Workshop	Speakers
10:00 AM – 4:30 PM	1. AI in Drug Discovery and Development	Dr Vinod Devaraj, Senior Scientist II, Schrodinger, Bangalore Dr Dileep Kumar, Assistant Professor - Sr Scale, Dept. of Pharmaceutical Chemistry, MCOPS, MAHE, Manipal
	2. Application of DoE in Pharmaceutical Development	Dr Usha Y Nayak, Professor, Dept. of Pharmaceutics, MCOPS, MAHE, Manipal
	3. Analytical Applications in Drug Discovery and Drug Delivery	Dr Gurubasavaraj HM, Principal Technical Support Specialist, Southern Region, Waters India Ms Dilshad Pullancheri, Sales Development Specialist, Waters India
	4. Polymerase Chain Reaction and its Applications	Dr Jesil A Mathew, Associate Professor, Dept. of Pharmaceutical Biotechnology, MCOPS, MAHE, Manipal
	5. Scientific Manuscript Preparation and Journal Selection	Dr Yogendra Nayak, Associate Professor, Dept. of Pharmacology, MCOPS, MAHE, Manipal

*Note: Only for Preconference Registered Delegates

Day 2: FRIDAY August 29, 2025

8:00 AM - 9:15 AM	Registration	Venue: Dr TMA Pai Hall, 2 nd Floor, KMC, MAHE, Manipal
Scientific Sessions		Venue: Dr TMA Pai Auditorium, 3 rd Floor, KMC, MAHE, Manipal
9:30 AM – 10:00 AM	Inauguration	Chief Guest: Dr H S Ballal, Pro Chancellor, MAHE Manipal
10:00 AM – 10:45 AM	Chairperson: Dr Manesh Thomas, Chief Executive Officer, Manipal - Government of Karnataka Biocubator, MAHE, Manipal	Speaker: Dr Sunil Kumar Panigrahi, Associate Vice President, Aurigene Pharmaceutical Services Limited, Bangalore Topic: From Lab to Clinic: Discovery of Potent and Selective PPAR δ Modulators
Tea Break		
11:00 AM – 11:45 AM	Chairperson: Dr Ramakrishna Shabaraya A, Principal, Srinivas College of Pharmacy, Mangalore	Speaker: Dr Kamal Dua, Associate Professor, University of Technology Sydney, Sydney, Australia Topic: Emerging Therapeutic Interventions in the Treatment of Lung Diseases: Discovery & Roadmap Through Interdisciplinary Research of Biological Advances to Advance Delivery Systems
11:45 AM – 12:30 PM	Chairperson: Dr Mohammed Gulzar Ahmed, Principal, Yenepoya Pharmacy College & Research Centre, Mangalore	Speaker: Dr Zohar Sihorwala, Senior Vice President & Head – Global Regulatory Affairs, Wockhardt Limited, Aurangabad Topic: The Role of Regulatory Affairs in Enabling Innovation and Access
Lunch Break		Venue: Dr TMA Pai Hall, 2 nd Floor, KMC, MAHE, Manipal
2:15 PM – 4:30 PM	Poster Presentations	Venue: Dr TMA Pai Hall, 1 st Floor, KMC, Manipal Session 1: 2:15 PM – 3:30 PM Session 2: 3:45 PM – 5:00 PM
6:30 PM – 8:00 PM	Entertainment Venue: Dr TMA Pai Auditorium, 3 rd Floor, KMC, MAHE, Manipal	
8:00 PM – 9:30 PM	Gala Dinner Venue: Dr TMA Pai Hall, 2 nd Floor, KMC, MAHE, Manipal	



MANIPAL PHARMACEUTICAL CONFERENCE

August 28-30, 2025

MPCON

2025

Theme
**Translating Innovation: Bridging Pharmaceutical Research
and Therapeutic Outcome**

PROGRAM SCHEDULE

Day 3: SATURDAY August 30, 2025

Venue: Dr TMA Pai Auditorium, 3rd Floor, KMC, MAHE, Manipal

9:15 AM – 10:00 AM	Chairperson: Dr Satish Rao , Director, Manipal School of Life Sciences, MAHE, Manipal	Speaker: Dr Abhijeet Pandey , Manager, R&D Competitive Intelligence, Novartis Healthcare Topic: Targeting Oligonucleotide to the Brain: Technology Intelligence and Landscape Analysis
10:00 AM – 10:45 AM	Chairperson: Dr Raviraja N S , Senior Director – Research, Directorate of Research, MAHE, Manipal	Speaker: Dr Praveen Kumar Shetty , Former Assistant Vice President-Clinical Development- Bioplus Life Sciences, Bangalore Topic: Endpoints in Clinical Trials for the Regulatory Approval of Oncology Molecules
	Tea Break	
11:00 AM – 11:45 AM	Chairperson: Dr Marina Koland , Principal, NGSM Institute of Pharmaceutical Sciences, Mangalore	Speaker: Dr Mahadev Rao , Professor, Department of Pharmacy Practice, Manipal College of Pharmaceutical Sciences, MAHE, Manipal Topic: The Significance of Translational Research in the Advancement of Precision Medicine in India
11:45 AM – 1:30 PM	PharmAZy Quiz Final Round Chairperson: Dr Paras Sharma , Associate Editor, Journal of Applied Pharmaceutical Science, New Delhi Quiz Master: Dr Jeyaprakash R S , Associate Professor, Dept. of Pharmaceutical Chemistry, MCOPS, MAHE, Manipal	
Lunch Break		
Venue: Dr TMA Pai Hall, 2 nd Floor, KMC, MAHE, Manipal		
2:30 PM – 3:30 PM	Panel Discussion Chairpersons: Dr Saleemulla Khan , Principal, P A College of Pharmacy, Mangalore Dr Prakash Goudanavar , Principal and Dean, Sri Adichunchanagiri College of Pharmacy, B G Nagar, Karnataka	Topic: AI and ML in Drug Discovery and Development Moderator: Dr Bharath B R , Senior Research Officer, Jai Research Foundation, Vapi, Gujarat Panelists: Dr Jagdish K , Vice President, Global Head - Healthcare and Life Sciences, Zensar Technologies, Hyderabad Dr R Govindarajan , Chief Innovation Officer, Adret Retail Ltd (Kapiva), Bangalore Dr Abhijeet Pandey , Manager, R&D Competitive Intelligence, Novartis Healthcare
3:30 PM – 4:30 PM	Prize Distribution and Valedictory	Chief Guest: Dr Sharath K Rao , Pro Vice Chancellor (Health Sciences), MAHE, Manipal
4:30 PM	High Tea	



Glimpses of MPCON 2025

MANIPAL PHARMACEUTICAL CONFERENCE 2025

August 28-30, 2025

MPCON

MPCON 2025 was successfully organized, drawing overwhelming participation from delegates, academicians, researchers, and students from across the country. The conference brought together over 500 delegates representing diverse disciplines within pharmaceutical sciences, creating a vibrant platform for knowledge sharing and networking. A total of 360 scientific posters were presented, showcasing innovative research in pharmacology, pharmaceuticals, biotechnology, pharmacognosy, pharmaceutical chemistry, quality assurance, and regulatory sciences.

The quiz competition saw enthusiastic participation, with five teams advancing to the finals. Scientific excellence was recognized through **42** awards, including Best Poster awards and **2** quiz awards. With its engaging sessions, interactive discussions, and active involvement from both students and faculty, MPCON 2025 emerged as a dynamic academic gathering that fostered learning, collaboration, and innovation in pharmaceutical sciences.



Chief Guests

**Chief Guest for
MPCON 2025 Inauguration**



Dr. H S Ballal
Pro Chancellor
MAHE, Manipal
Karnataka

**Chief Guest for
MPCON 2025 Valedictory**



Dr. Zoher Sihorwala
Senior Vice President and Head
Global Regulatory Affairs Wockhardt
Limited, Maharashtra

**Chief Guest for
MPCON 2025 Preconference Workshop**



Dr. Anil K Bhat
Dean
KMC,MAHE,
Manipal

Chairpersons



Dr. Manesh Thomas
Chief Executive Officer
(CEO)
BioNEST, MAHE, Manipal,
Karnataka



**Dr. Ramakrishna
Shabaraya A**
Professor & Principal
Srinivas College of
Pharmacy, Valachil,
Mangalore



**Dr. Mohammed
Gulzar Ahmed**
Principal & Dean
Yenepoya Pharmacy College &
Research Centre,
Mangalore



Dr B S Satish Rao
Director
Manipal School of
Life Sciences
MAHE, Manipal



Dr Saleemulla Khan
Principal
P A College of Pharmacy
Mangalore



Dr Marina Koland
Principal
NGSM Institute of
Pharmaceutical Sciences,
Mangalore



Dr Paras Sharma,
Associate Editor,
Journal of Applied Pharmaceutical
Science
New Delhi



Dr Raviraja N S
Senior Director Research
Directorate of Research
MAHE, Manipal



Dr. Prakash S Goudanavar
Principal & Dean
Faculty of Pharmacy
Adichunchanagiri University
B.G.Nagara

Speakers



Dr. Sunil Kumar Panigrahi

Associate Vice President, Aurigene Pharmaceutical Services Limited, Bengaluru

Topic: : From Lab to Clinic: Discovery of Potent and Selective PPAR δ Modulators



Dr Kamal Dua

Associate Professor, University of Technology Sydney, Australia

Topic: Emerging therapeutic interventions in the treatment of lung diseases: Discovery & roadmap through an interdisciplinary research of biological advances to advance delivery systems



Mr. Zoher Sihorwala

Senior Vice President & Head, Global Regulatory Affairs, Wockhardt Limited, Maharashtra

Topic: : The Role of Regulatory Affairs in Enabling Innovation and Access



Dr. Abhijeet Pandey

Manager, R&D Competitive Intelligence, Novartis Healthcare

Topic: : Targeting Oligonucleotide to Brain



Dr. Praveen Kumar Shetty

Assistant Vice President-Clinical Development- Bioplus Life Sciences, Bangalore

Topic: : Determining Appropriate Endpoints in Oncology Clinical Trials



Dr. Mahadev Rao

Professor, Department of Pharmacy Practice MCOPS, MAHE Manipal

Topic: : The significance of translational research in the advancement of Precision Medicine in India



Dr. Bharath BR

Senior Research Officer, Jai Research Foundation, Vapi, Gujarat

Moderator of Panel Discussion on AI and ML in Drug Discovery and Development



Dr. Jagdish . K

VP Global Head Healthcare & Life Sciences, Zensar Technologies, Hyderabad

Topic: : AIML GenAI in Pharmaceutical Industry



Dr. R Govindarajan

Chief Innovation Officer, Adret Retail Ltd (Kapiva), Bangalore

Topic: : AI in Natural Products Drug Discovery and Development

Preconference Workshop

Resource Persons



Dr. Vinod Devaraj

Senior Scientist II
Schrödinger,
Bangalore



Dr. Usha Y Nayak

Vice Principal and Professor,
Dept. of Pharmaceutics,
MCOPS, MAHE, Manipal



Dr. Yogendra Nayak

Associate Professor
Dept. of Pharmacology,
MCOPS, MAHE, Manipal



Dr. Gurubasavaraj HM

Principal Technical Support Specialist
Southern Region, Waters India



Ms. Dilshad Pullancheri

Sales Development Specialist
Waters India



Dr Kiran Kumar Kolathur,

Assistant Professor-Senior Scale,
Department of Pharmaceutical Biotechnology,
MCOPS, MAHE Manipal



Dr. Dileep Kumar

Assistant Professor – Sr Scale
Dept. of Pharmaceutical Chemistry,
MCOPS, MAHE, Manipal

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Manipal College of
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Vice-Principal & Professor
Manipal College of
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Dr. Nandhakumar K
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Department of Pharmacology

Hospitality & Transportation Committee



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Additional Professor & Head
Department of
Pharmaceutical Chemistry

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Professor & Head
Department of Pharmaceutics

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Associate Professor & Head
Department of Pharmacognosy

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Dr. M Surulivel Rajan
Professor & Head
Department of Pharmacy Practice

MPCON 2025 List of Volunteers

Registration and Poster sessions

Faculty coordinators: Dr Muddukrishna and Dr Anoop Kishore

Department	Research Scholars
Pharmaceutics	Abhijith K Shaji
	Devika Sajeev
	Raagul S
	Tamizharasan A
	Anoushka
	Sandesh
	Mahesha
Pharmacology	Vishwani
	Pratyasha
	Sandra
	Niyogitha
	Manjunath
	Raghavendra
	Ishwar
Quality Assurance	Tanvi
	Supraja
	Roshan
	Suyash
Pharmacognosy	Megha
	Vijishna

MPCON 2025 List of Volunteers

Inaugural, Oral Scientific Sessions and Valedictory sessions

Faculty Coordinators: Dr Shaila and Dr Yogendra Nayak

Pharmacology	Vishnusai
Pharmaceutical Biotechnology	Navas Sherif
	Rafwana
	Sanskriti Patil
	Rahul
RA and management	Anusha Prabhu
	Pooja

Food and Hospitality committee volunteers

Faculty coordinator: Dr Varadraj Bhat

Pharmacy Practice	Sushant
	Zuha Shyma
	Sai
Pharmaceutical Chemistry	Pratyashok Dash
	Giridhar Jyothi
	Stutee Das
	Tisa Francis
	Sai Nikhil
	Shareef Shaik

Print and Media

Faculty coordinator: Dr Vasudev Pai

Pharmacy Practice	Sushant
	Zuha Shyma
	Sai

Schedule of Poster Presentations

Date: 29 Aug 2025

Venue: Dr TMA Pai Auditorium, KMC, MAHE, Manipal

Session	Poster category	Poster ID codes	Page number
Session – I 2.00 pm to 3.30 pm	Pharmaceutics, Drug Delivery and Biopharmaceutics	PD-DB-001 to PD-DB-105	1-107
	Drug Regulatory Affairs and Pharmaceutical Management	DRA-PM-001 to DRA-PM-055	108-169
	Pharmaceutical Analysis and Quality Assurance	PA-QA-001 to PA-QA-025	170-194
	Pharmacognosy and Phytomedicine	PCO-PM-001 to PCO-PM-018	195-215
Session – II 3.45 pm to 5.15 pm	Pharmacology and Biotechnology	PHA-BT-001 to PHA-BT-088	216-306
	Pharmaceutical Chemistry and Drug Discovery	PC-DD-001 to PC-DD-066	307-375
	Pharmacy Practice and Clinical Pharmacy	PP-CP-001 to PP-CP-035	376-409

Abstracts

Category 1

Pharmaceutics, Drug Delivery and Biopharmaceutics

- 1 -



PD-DB-001: Formulation and Characterization of Phytosomes loaded Anti-Fungal Emulgel from the leaf extract of *Psidium guajava* L.

Rohithkumar C¹, Aiswarya K N²

¹Department of Pharmaceutics, KMCH College of pharmacy, Coimbatore-641048, Affiliated to The Tamil Nadu Dr.M.G.R. Medical University, Tamil Nadu, India.

² Faculty of Pharmacy, Karpagam Academy of Higher Education, Coimbatore-641021, Tamil Nadu, India

Rohithkumarc29@gmail.com

Background: *Psidium guajava* L. (guava) leaves are widely recognized for their antimicrobial and antioxidant properties, but their therapeutic potential is limited by poor solubility and bioavailability. Phytosome technology offers an innovative approach to enhance the delivery and effectiveness of plant-derived bioactives in topical applications. This study aimed to develop and evaluate a phytosome-based antifungal emulgel incorporating guava leaf extract to improve topical drug delivery and therapeutic efficacy.

Methods: Phytosomes were prepared via rotary evaporation using guava leaf extract and soya lecithin in molar ratios of 1:1, 1:2, and 1:3. The optimized formulation (F2) was incorporated into an emulgel base. The formulation was evaluated for particle size, zeta potential, entrapment efficiency, FTIR, TEM, pH, spreadability, swelling index, in vitro drug release, and antifungal activity against *Candida albicans* using the agar well diffusion method.

Results: The F2 formulation showed optimal particle size, high entrapment efficiency, and good stability. The phytosomal emulgel demonstrated suitable pH, spreadability, and swelling behavior. *In vitro* studies confirmed sustained drug release, while antifungal testing indicated significantly enhanced inhibition compared to conventional formulations.

Conclusion: The developed phytosomal emulgel of *Psidium guajava* leaf extract effectively improved antifungal activity and bioavailability, suggesting its potential as a promising topical herbal therapy.

Keywords: *Psidium guajava*, phytosomes, emulgel, antifungal activity, topical delivery, bioavailability



PD-DB-002: Comparative study of modified polymers for buccal drug delivery of carvedilol

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Background: Carvedilol, a non -selective β -adrenergic blocking agent is a vasodilator act by blocking the activity of alpha-1 receptors indicated for the chronic therapy of heart failure, left ventricular dysfunction, myocardial infarction. The drug is well absorbed on oral administration, but its bioavailability is low (25-35%) due to first pass metabolism. To overcome this problem buccal drug delivery is used, which is a promising alternative route for systemic drug administration.

Aims & Objectives: The study was aimed at comparative assessment of natural polymers and their derivatives for the use in buccal drug delivery.

Methods: Thiolated derivatives of the polymers were synthesized using carbodiimide and hydrochloric acid, and thiol group conjugation. The tablets were prepared by direct compression where polymers, drug and excipients in different ratio were added, mixed and compressed on a single station punching machine. Eight different formulations were evaluated for physicochemical properties, in vitro drug release, in vitro permeation, bio adhesive strength, and in vitro residence time.

Results: The formulations were prepared using sodium alginate and chitosan providing drug release of 55.53 ± 0.28 to 70.86 ± 0.49 and 32.80 ± 0.41 to 57.89 ± 0.44 respectively. Formulation containing modified alginate and chitosan exhibited release of 64.59 ± 0.4 to 74.24 ± 0.44 and 53.18 ± 0.44 to 72.23 ± 0.32 respectively the prepared tablet had a hardness of 5.03 ± 0.30 to 7.3 ± 0.36 . The bioadhesion strength of tablet for sodium alginate and chitosan was 13.9 ± 0.65 and 23.93 ± 0.4 . Whereas the modified alginate chitosan showed and increased bio adhesion strength that is 18.56 ± 0.81 and 34.28 ± 0.91 .

Conclusion: Thiolated polymers significantly improve the performance of buccal mucoadhesive tablets of carvedilol, making them a suitable strategy for effective buccal drug delivery.

Keywords: Buccal drug delivery, sodium alginate, pectin, chitosan, xanthan gum, thiolation, mucoadhesion, buccal tablets.



PD-DB-003: Design, development and characterisation of voriconazole niosomal gel

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The aim of our study is to design and develop and characterize Voriconazole Niosomal gel. The objective for current study is to develop a drug encapsulation system in niosome vesicles for the successful topical drug delivery and to develop Niosomal Voriconazole Gel for effective treatment of topical fungal infections by enhancing its permeation and bioavailability of the drug. The method used to prepare Voriconazole Niosomal Gel for management of antifungal infections like *Invasive Candida infection*, *Invasive Aspergillus* is by ether injection method. The drug mixtures compatibility were determined by FTIR, found to be compatible with each other. The developed niosomes formulation, were optimized based upon the evaluation parameters such as Particle size, Zeta potential, Drug entrapment, and Drug content. The particle size range of the prepared niosomes are in the nano-size range. From the results of above evaluation studies, Formulation F1 was optimized, whose particle size are in the range of 27.74 nm. So, the formulation F1 has been converted into gel. In-vitro drug release of formulation F1 had exhibit release profile of 83.67% and it had followed zero- order kinetics. The stability testing of the optimized preparation was also observed to be satisfactory. The niosomal vesicle represented to be an efficient nano vesicular carrier, to decrease the therapeutic dose of Voriconazole gel by improving its performance.

Keywords: Niosomes, Voriconazole, Nano-size, Gel, Antifungal activity.



PD-DB-004: Design and optimization of spray-dried unloaded liposomes as a flexible drug carrier

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Liposomes are recognized as versatile nanocarriers due to their biocompatibility, structural flexibility, and capacity to encapsulate both hydrophilic and lipophilic drugs. Spray-dried unloaded liposomes offer a promising foundation for various drug delivery applications, supporting controlled release and enhanced stability. These liposomes are prepared using soybean phosphatidylcholine and cholesterol in optimized ratios via thin-film hydration followed by sonication and spray drying. The incorporation of carbohydrate-based excipients such as mannitol improves structural integrity during the drying process and enhances reconstitution efficiency. Optimization through a Quality-by-Design (qbd) approach enables precise control over critical parameters including particle size, Polydispersity Index (PDI), Percentage yield, and Encapsulation potential. Structural using FTIR confirms formulation stability. Upon reconstitution, the liposomes maintain uniform morphology and long-term stability, making them suitable for future drug loading. A model drug, Atorvastatin, demonstrates sustained in vitro release when loaded into the liposomes, validating their potential for controlled drug delivery. The spray-dried form offers key advantages such as extended shelf life, reduced aggregation, and improved handling, making this platform ideal for oral, pulmonary, injectable, and targeted delivery systems. Overall, spray-dried unloaded liposomes present a scalable, cost-effective, and customizable approach for developing advanced pharmaceutical formulations.

Keywords: Spray-dried liposomes, unloaded liposomes, phosphatidylcholine, cholesterol, nanocarrier, controlled release, qbd, trehalose, atorvastatin, drug delivery.



PD-DB-005: Green Synthesis of *Wrightia tinctoria* R. Br Leaf Extract Zinc Oxide Nanoparticles Embedded Nanoemulgel as a Paradigm for Treatment of Psoriasis

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Psoriasis is a chronic, relapsing inflammatory skin disorder with limited therapeutic options and considerable side effects from conventional treatments. This research aims to develop a safe, plant-based nanocarrier system using green synthesis for effective topical management of psoriasis. Zinc oxide nanoparticles (zno-nps) were synthesized using the ethanolic leaf extract of *Wrightia tinctoria* R.Br, a medicinal plant known for its anti-inflammatory and wound-healing properties. The synthesized zno-nps were characterized using UV-Vis spectroscopy, FTIR, XRD, and particle size analysis. The zno-nps were then incorporated into an optimized Nano emulsion system and formulated into a Carbopol-based nanoemulgel. The final formulation was evaluated for physicochemical properties such as pH, viscosity, spreadability, homogeneity, and drug content. In vitro diffusion studies showed sustained release of the active compounds, while antioxidant assays confirmed free radical scavenging potential. Acute dermal toxicity studies were conducted following OECD guideline 402 using female Wistar albino rats to assess the safety of the nanoemulgel. No signs of toxicity, erythema, or edema were observed, confirming the formulation's dermal safety. Additionally, in vivo anti-psoriatic activity was evaluated using the imiquimod-induced psoriasis-like plaque model in Wistar rats. The nanoemulgel-treated group showed significant improvement in Psoriasis Area Severity Index (PASI) scores, reduction in epidermal thickness, and histopathological improvement compared to the control. This study concludes that *Wrightia tinctoria*-based zno nanoparticle-embedded nanoemulgel is a promising and safe green nanotherapeutic strategy for the effective topical treatment of psoriasis.

Keywords: *Wrightia tinctoria*, Zinc oxide nanoparticles, Nanoemulgel, Green synthesis, Psoriasis, Acute dermal toxicity, Wistar rats, In vivo model



PD-DB-006: Formulation of aceclofenac loaded film forming gel for topical pain management.

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Background: Topical delivery of NSAIDs provides targeted pain relief with fewer systemic side effects. Film-forming gels offer sustained drug release, better skin adherence, and improved patient comfort. Aceclofenac is a suitable candidate for such delivery systems in managing long-term topical pain.

Aims & Objectives: To develop a aceclofenac-loaded film-forming gel (FFG) with the target of providing long-term topical pain relief and continuous drug release upon application.

Methods: ffgs were prepared using drug, chitosan, hydrophilic polymer, plasticizer, water, and ethanol by simple mixing. The primary mechanical properties were evaluated by film formation time, tensile strength, and break elongation. Skin permeation of the drug was identified by an in vitro skin permeation study conducted using a Franz diffusion cell with a synthetic membrane.

Results: The FFG exhibited good film formation, ranging from 7–8 minutes. The film demonstrated good flexibility upon drying after application to the skin, with minimal to no detectable odour. It did not adhere to clothing and could be easily removed using plain water.

Conclusion: These properties suggest its potential as a promising alternative for long-term topical pain management.

Keywords: Aceclofenac, film-forming gel, chitosan, topical pain relief, skin permeation, Franz diffusion cell.



PD-DB-007: Evaluation of antimicrobial effect of herbal ointment containing extracts of *tagetes erecta* (marigold) and *Caesalpinia Pulcherrima* (peacock flower)

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Aim: This study investigates the antimicrobial properties of herbal ointments formulated with ethanolic extracts of *Tagetes erecta* (Marigold) and *Caesalpinia pulcherrima* (Peacock flower).

Methods: The extraction process involves maceration of fresh plant materials in ethanol, followed by filtration and concentration to obtain thick extracts rich in bioactive compounds. The ointment formulation incorporated cetyl alcohol, beeswax, white soft paraffin, and the plant extracts in specific proportions to achieve the desired consistency. Preliminary phytochemical screening was conducted to identify key constituents such as alkaloids, flavonoids, tannins, and triterpenes. The evaluation methods included visual assessment, pH measurement, spreadability testing, and antimicrobial susceptibility testing against Gram-positive bacteria (*Staphylococcus aureus*, *Bacillus subtilis*) and Gram-negative bacteria (*Pseudomonas aeruginosa*, *Escherichia coli*).

Results: The phytochemical analysis showed that *Tagetes erecta* contains alkaloids, triterpenes, tannins, and flavonoids, while *Caesalpinia pulcherrima* has only tannins and flavonoids. The herbal ointment has a greenish colour, aromatic odour, neutral pH (7), and is non-irritant and easily spreadable. In antimicrobial tests, it exhibited inhibition zones of 11 mm for *Staphylococcus aureus*, 40 mm for *Bacillus subtilis*, 3 mm for *Pseudomonas aeruginosa*, and 4 mm for *Escherichia coli*, indicating varying antimicrobial activity.

Conclusion: The study confirms that an ointment containing ethanolic extracts of *Tagetes erecta* and *Caesalpinia pulcherrima* effectively inhibits gram-positive bacteria and can be used topically to protect the skin. The presence of active compounds like alkaloids and flavonoids supports its antibacterial properties, highlighting its potential as a medicinal treatment against antibiotic-resistant pathogens.

Keywords: Herbal ointment, antimicrobial activity, irritancy, spreadability.



PD-DB-008: Solubility enhancement of rosuvastatin using co-crystal approach

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Rosuvastatin has been used to commercially treat hyperlipidaemia by reducing triglycerides, apolipoprotein and low-density lipoproteins and increasing high-density lipoproteins and decreasing triglycerides. However, it is a BCS class II drug and has the problems of low aqueous solubility and low bioavailability. The cocrystal approach has been repeatedly used to improve the solubility of poorly soluble drugs, while showing potential to improve other physicochemical properties. The cocrystal approach also shows a high degree of dependence on the manufacturing methods used to produce the same. In this study, cocrystals of Rosuvastatin calcium have been synthesized using the amino acid cofomers L-Glutamine and L-Asparagine. These cocrystals have been produced using two separate manufacturing techniques which are spray drying and solvent evaporation respectively. Solubility studies were used to identify the manufacturing technique with better solubility parameters. Solid state characterization like Fourier-Transform Infrared Red spectroscopy, Differential Scanning calorimetry and Powder X-Ray Diffraction studies were performed on the shortlisted cocrystals and dissolution studies were conducted to quantify the solubility enhancement observed by cocrystallization.

Key words: RSC: Rosuvastatin calcium, BCS: Biopharmaceutical classification system, SE: Solvent evaporation, SD: Spray drying, PXRD: Powder X-Ray Diffraction, DSC: Differential Scanning Calorimetry, FTIR: Fourier Transform Infra-Red Spectrophotometry, cocrystal G: Glutamine cocrystal, cocrystal A: Asparagine cocrystal.



PD-DB-009: Formulation and Evaluation of a Mucoadhesive Drug Delivery System Incorporating Nanosuspension of Cinnarizine

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Background: Cinnarizine, a BCS Class II antihistaminic used for motion sickness and vertigo, shows poor aqueous solubility and low oral bioavailability, leading to inconsistent absorption. Also it has absorption window in stomach. Conventional formulations often require higher doses, increasing the risk of side effects. Nanosuspension technology offers a promising approach to enhance solubility, dissolution, and bioavailability of such poorly soluble drugs.

Aims & Objectives: To formulate and evaluate a nanosuspension of Cinnarizine using media milling, aimed at increasing aqueous solubility and improving oral bioavailability.

Methods: Cinnarizine nanosuspension was prepared using zirconium oxide beads. HPMC E5 was used as stabilizer and poloxamer as surfactant. Gastro retentive hydrogels were prepared using carbopol and HPMC. The formulation was evaluated for particle size, zeta potential, drug content, in-vitro drug release and permeation.

Results: The nanosuspension showed particle sizes ranging from 444 to 919 nm, and zeta potential from -17.3 to 32.7 mv. The mucoadhesive gel containing nanosuspension (CG1) released 84.4% of drug in 6 hours in 0.1 N hcl. Drug release followed first-order kinetics and case-II transport.

Conclusion: CG1 formulation demonstrated improved solubility, controlled drug release, and potential enhancement in bioavailability.

Keywords: Cinnarizine, media milling, nanosuspension, zirconium beads, HPMC, mucoadhesive gel.



PD-DB-010: Encapsulation of papain and cinnamon oil in pectin based herbal periodontal films for treatment of periodontitis

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Background: Periodontitis is a serious gum infection that damages the soft tissue and bone supporting the teeth. While conventional treatments often rely on antibiotics, these can lead to side effects and antibiotic resistance. There is a growing need for safe, localized alternatives that can effectively manage the infection and inflammation associated with this condition.

Aims & Objectives: This study focuses on developing herbal periodontal films using natural ingredients papain and cinnamon oil embedded in a pectin base. The goal is to create a biocompatible film that can adhere to the gums, release the actives gradually, and help reduce infection and inflammation directly at the site.

Methods: The films were prepared using the solvent casting technique, with papain and cinnamon oil incorporated into a pectin matrix. The formulations were optimized using Design Expert® software and evaluated for physical properties, drug content, *in-vitro* drug release, antibacterial activity, and safety through cell-line studies including MTT, Crystal Violet, and TLR-4 assays.

Results: The optimized films showed good strength, sustained drug release, and effective antibacterial action against *S. Aureus* and *E. Coli*. Cell-line studies confirmed that the films were safe and demonstrated strong anti-inflammatory activity.

Conclusion: These herbal periodontal films offer a gentle, targeted approach to treating periodontitis. By combining natural activities with a modern delivery system, this formulation provides a promising alternative to conventional therapies.

Keywords: Periodontitis, Herbal periodontal film, Papain, Cinnamon oil, Pectin, Localized therapy, Anti-inflammatory, Antibacterial, Biocompatible film, Drug release.



PD-DB-011: Investigation on multifunctional nanotheranostic platform against glioblastoma via direct nose-to-brain delivery

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Background: Glioblastoma (GBM) is a highly aggressive form of brain cancer that stands difficult to treat, particularly due to a lack of effective targeting and drug delivery possibilities. Because of its anatomical benefits, the nose-to-brain method is an intriguing route for medication administration. Nanoengineering has offered technical tools and novel ways to conquer biotechnological restrictions, which holds promise for boosting the efficacy of traditional medicines.

Methods: Herein, we designed a multifunctional theranostic nanoparticles produced by polymeric (PLGA)-core co-loaded with zns@CMC qds and Chrysin (CHR) and further coated with folate- trimethyl chitosan (Fol-TMC) conjugate as a targeting ligand. The developed nanoparticles Fol-TMC-(zns@CMC, CHR)-nps were extensively characterized, and their biological performance was investigated.

Results: The results indicate that nps could control CHR release and promote CHR permeation across the sheep nasal mucosal membrane ex vivo. The higher cytotoxicity of nps in glioma (U87MG) cell line reinforces their potential for targeting the folate receptor overexpressed on GBM tumor cells. In vivo biodistribution studies showed that the fabricated nps effectively reach the brain following intranasal administration, and CLSM data indicated the high cellular uptake of the nps.

Conclusion: These findings suggest that nps hold promise as a bioimaging nanoplatform for effectively targeting the GBM tumor and present a high potential for clinical translation.

Keywords: PLGA: poly(D, L-lactic-co-glycolic) acid; CHR: Chrysin; zns qds: Zinc sulfide quantum dots; Fol: Folate; TMC: N,N,N-trimethyl chitosan; CLSM: Confocal laser scanning microscopy; nps: Nanoparticles; GBM: Glioblastoma



PD-DB-012: Development and Evaluation of Eberconazole-Loaded Nanoemulgel for Dermal Application.

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Background: Eberconazole, a broad-spectrum imidazole antifungal, requires an effective delivery system to enhance its therapeutic efficacy. Topical antifungal therapy often suffers from poor drug penetration and low skin retention. Nanoemulgels, which combine the benefits of nanoemulsions and gels, offer a promising strategy for improved topical delivery by enhancing drug solubility and stability.

Aims & Objectives: The aim of this study was to develop and evaluate a nanoemulgel formulation of eberconazole to enhance its topical delivery and antifungal effectiveness

Methods: Drug solubility studies were conducted in various oils, surfactants, and co-surfactants to identify optimal components. Almond oil was selected as the oil phase, Span 20 as the surfactant, PEG 400 as the co-surfactant, and distilled water as the aqueous phase. Nanoemulsions were prepared using the ultrasonic emulsification method. Formulations were evaluated for particle size, polydispersity index (PDI), and zeta potential. The optimized nanoemulsion was incorporated into a gel base (Carbapol 934) to form the nanoemulgel. The nanoemulgel were characterized for various physicochemical parameters. The in vitro drug diffusion studies were performed to assess drug release from the prepared formulations.

Results: The optimized nanoemulsion comprised 1% almond oil, 0.6% Span 20, 0.2% PEG 400, and 0.4% water. It demonstrated a mean globule size of 387.3 nm, a PDI of 0.492, and a zeta potential of -29.5 mv. The nanoemulgel showed a drug release of $15.29 \pm 0.20\%$ over 6 hours, indicating sustained release characteristics. Drug content was found to be 102.42 ± 1.34 $\mu\text{g/ml}$.

Conclusion: The formulated eberconazole nanoemulgel demonstrated suitable physicochemical properties and sustained drug release, making it a promising approach for the improved topical treatment of fungal infections. The formulation strategy may enhance skin drug penetration and therapeutic efficacy.

Keywords:

Eberconazole, nanoemulsion, penetration enhancement, topical anti-fungal, gel.



PD-DB-013: Formulation and evaluation of transdermal patches of Carvedilol using natural polymer obtained from fruits of *Ficus auriculata* (Lour)

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Background: Transdermal drug delivery systems (TDDS) have emerged as a promising alternative to oral administration by enabling sustained drug release and enhancing patient compliance. Carvedilol, a non-selective beta-blocker used in the treatment of hypertension and heart failure, suffers from low oral bioavailability due to extensive first-pass metabolism. Natural polymers, such as *Ficus auriculata* mucilage, have gained interest due to their biocompatibility, biodegradability, and excellent film-forming properties.

Aim and Objectives: This study aimed to extract and evaluate mucilage from *Ficus auriculata* fruits. The transdermal patches of Carvedilol will be formulated using the mucilage. The compatibility studies will be performed using FTIR. The patches will be evaluated for physical, drug release characteristics, and stability.

Methods: Mucilage was extracted from the fruit pulp of *Ficus auriculata* and evaluated for physicochemical properties. Transdermal patches were prepared with varying drug concentrations of *Ficus auriculata* mucilage and PVA. The formulations were assessed for compatibility, thickness, folding endurance, moisture content, drug content, stability study, and in vitro drug release using a Franz diffusion cell over 8 hours.

Results: The extracted mucilage was found to have good film-forming properties. FTIR confirmed the compatibility between the drug and the extracted natural polymer. All patches were uniform, smooth, and had good folding endurance. Among the prepared formulations, formulation F3 demonstrated the best sustained-release profile, releasing $54.05 \pm 0.20\%$ of the drug over 8 hours. As the polymer ratio increases, drug release decreases.

Conclusion: The results showed that the transdermal patches were successfully prepared for carvedilol formulated using *Ficus auriculata* mucilage.

Keywords: Carvedilol, Transdermal patches, *Ficus auriculata* mucilage, solvent casting, Natural polymer



PD-DB-014: Papain-Loaded Film-Forming Spray: A Stable and Effective Topical Therapy for Gingivitis with Dual Anti-Inflammatory and Antimicrobial Action

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This study presents the development and evaluation of a Papain-Loaded film-forming spray (FFS) for gingivitis treatment. The spray was formulated using papain and propylene glycol in a solvent blend, with Eudragit and HPMC as polymers, yielding a homogeneous solution suitable for oral application. Physicochemical analyses, including FTIR and SEM, confirmed the chemical stability and uniform film morphology essential for consistent drug delivery. The optimized formulation demonstrated a viscosity of 13.18 cps and a pH of 6.74, aligning with oral mucosa tolerance. The spray exhibited rapid film formation (92.33 seconds), wide spray coverage (15.43 cm pattern, 52.38° angle), and good sprayability due to its low density (0.508 g/ml). In vitro studies revealed 86.83% drug permeation and sustained antimicrobial efficacy against both Gram-positive and Gram-negative bacteria, with peak inhibition at 48 hours. Stability testing over two months showed no significant changes in key parameters. Biocompatibility was confirmed by dual cytotoxicity assays, maintaining cell viability above 95%. Mechanistic studies demonstrated dual anti-inflammatory action: papain's proteolytic activity and modulation of the TLR-4/myd88/NF- κ B pathway, with significant reductions in pro-inflammatory cytokines and TLR-4 expression. The spray accelerated resolution of inflammation compared to controls. These results indicate that the papain-loaded FFS is a stable, safe, and effective topical therapy for gingivitis, offering rapid film formation, sustained drug release, and significant anti-inflammatory and antimicrobial effects, positioning it as a promising adjunct for oral care and periodontal disease management.

Keywords: Papain (PAP), Film-Forming Spray (FFS), Gingivitis (GIN), Eudragit (EUD), Hydroxypropyl Methylcellulose (HPMC), Antimicrobial Activity (AMA), Anti-Inflammatory (AIF), TLR-4/myd88/NF- κ B Pathway (TLR-4), Cytotoxicity Assay (CTA), Oral Drug Delivery (ODD)



PD-DB-015: Development of solid lipid nanoparticles of curcumin

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Background: Curcumin has excellent anti-inflammatory activity and antimicrobial activity relevant to acne treatment. However, due to its poor aqueous solubility and photodegradability, curcumin is seldom used clinically. To overcome these problems, solid lipid nanoparticles (SLN) are selected for the effective delivery of curcumin for acne.

Aims & Objectives: The aim of the study was to develop curcumin loaded solid lipid nanoparticle to deliver the drug to the acne site.

Methods: Screening of lipids were carried out and solubility of curcumin in different lipids and surfactants was evaluated. Based on the preliminary study, a combination of compritol and PVA was selected as lipid and surfactant. The SLN's were prepared by hot emulsification/ultra-sonication method with drug to lipid ratio (0.25:1). The effect of process variables on nanoparticle characters were investigated. The prepared SLN's were evaluated for physico-chemical properties including drug release studies.

Results: The prepared SLN's had a particle size of 256.5 nm to 699.2 nm, zeta potential of -26.2mv to -2.03mv, PDI from 0.123 to 0.717 and an entrapment efficiency of 43.6 ± 0.40 to 71.6 ± 0.26 %. The SLN's released $4 \pm 0.5\%$ and $19 \pm 0.5\%$ in 8h. The drug release followed first order kinetics and non-fickian diffusion mechanism. The DSC results exhibited no interaction between curcumin and compritol. The results of XRD studies confirmed the crystalline state of drug, lipid and the formulation. The SLN's were spherical in shape as evidenced from SEM images.

Conclusion: The stability of curcumin can be enhanced significantly by formulating into SLN. The size of the formulation being in nano range offer enhanced therapeutic effectiveness of curcumin.

Keywords: Curcumin, solid lipid nanoparticle, hot emulsification/ultra-sonication method, compritol.



PD-DB-016: Formulation and evaluation of topical film forming Hydrogel containing amoxicillin loaded silver Nanoparticles for the treatment of wound infections

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Background: Wound infections remain a major healthcare challenge, further intensified by rising antimicrobial resistance, calling for innovative treatment approaches.

Aims & Objectives: To develop and evaluate a novel topical film-forming hydrogel incorporating Amoxicillin-loaded silver nanoparticles for enhanced wound healing and antimicrobial efficacy.

Methods: The formulation involved two concentrations of Amoxicillin-loaded silver nanoparticles (5 mg/ml and 10 mg/ml). Preformulation studies included compatibility checks via FTIR and confirmation of pharmacopeial standards. The physicochemical properties, entrapment efficiency, pH, viscosity, film formation, spreadability, and gel fraction were assessed. In vitro drug release (Korsmeyer-Peppas model), antimicrobial activity, cytotoxicity (L929 fibroblast cells), and in vivo wound healing in Wistar albino rats were studied. Histopathology and stability tests validated the outcomes.

Results: The 10 mg/ml nanoparticle hydrogel showed superior nanoscale particle size (52.6 nm), high entrapment efficiency, and favorable gel characteristics. It demonstrated sustained drug release over 24 hours and potent antimicrobial action against *S. Aureus*, *S. Pneumoniae*, *E. Coli*, and *P. Aeruginosa*. Cytotoxicity tests confirmed safety, and in vivo studies showed enhanced wound healing supported by histopathology.

Conclusion: The developed hydrogel offers a safe, biocompatible, and effective wound treatment with synergistic antimicrobial action and sustained drug delivery, addressing the challenges posed by resistant infections.

Keywords: Topical hydrogel, Amoxicillin, Silver nanoparticles, Wound healing, antimicrobial resistance, Sustained release, Biocompatibility



PD-DB-017: Design and evolution of Gastroretentive system of Famotidine

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Background: Oral delivery of drugs with a narrow absorption window, such as famotidine, can benefit from gastroretentive systems to enhance bioavailability and therapeutic efficacy. Hydrodynamically balanced systems (HBS) are an effective approach to prolong gastric residence time and achieve controlled drug release. These floating tablets remain buoyant in the stomach, allowing sustained and localized drug action. Hydroxypropyl methylcellulose (HPMC) is a commonly used polymer in such systems for controlling drug release.

Aims & Objectives: To develop and evaluate hydrodynamically balanced floating tablets of famotidine to prolong gastric residence time and sustain drug release.

Methods: Floating famotidine tablets were formulated using HPMC via direct compression, with variations in drug-to-polymer ratios and sublimating agents. The tablets were evaluated for physicochemical properties, drug-polymer compatibility, floating behaviour, drug release, and short-term stability. Results showed that drug release depended on the polymer ratio, and most formulations had a buoyancy lag time under 10 minutes and floated for over 24 hours.

Results: All formulations showed satisfactory physicochemical properties. The drug release rate was significantly influenced by the drug-to-polymer ratio, with higher polymer content leading to more sustained release. The floating ability was dependent on the type and amount of sublimating agent. Most formulations had a buoyancy lag time <10 minutes and remained buoyant for over 24 hours. Stability studies indicated no significant changes in drug content or floating behaviour over the testing period.

Conclusion: The developed hydrodynamically balanced famotidine tablets demonstrated prolonged gastric residence and sustained drug release. HPMC effectively controlled drug release, while the use of appropriate sublimating agents ensured rapid and sustained buoyancy. These results support the potential of HBS as a gastroretentive drug delivery system for famotidine.

Keywords: Hydrodynamically balanced system, Famotidine, Hydroxypropyl methylcellulose, Invitro floating, Sublimating agents



PD-DB-018: Computational Prediction of sirna Candidates for a Novel Therapeutic Strategy Against HSV-1

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Herpes Simplex Virus-1 (HSV-1) is a prevalent human pathogen affecting nearly 3.8 billion people under the age of 50 globally. It causes a range of infections, primarily recurrent vesicular eruptions in the orolabial and genital mucosa, to life-threatening encephalitis. Despite the availability of antiviral therapies, the emergence of resistant HSV-1 strains and the inability of treatments to eradicate and act against the latent virus highlight the need for novel therapeutic strategies. RNA interference (RNAi), particularly small interfering RNA (siRNA), offers a promising approach for silencing essential viral genes and inhibiting viral replication. We used in silico tools to design and screen siRNA candidates targeting conserved regions of essential HSV-1 genes, as well as the main genes involved in the disease progression. In addition to the essential genes, we also aimed to design the siRNA candidates targeting conserved regions of HSV-1 glycoprotein genes such as gB, gC, and gD, which play important roles in viral entry and immune evasion. The siRNAs were evaluated using GC content analysis, thermodynamic stability, and off-target analysis using BLAST against the human transcriptome. The top candidates were modelled for interaction with mRNA target using HnAdock to ensure efficient gene silencing. Our computational analysis led to the identification of 5 promising targets: ICP0, ICP4, ICP27, UL30, and UL18. The targets showed high specificity, strong thermodynamic stability, with minimal off-target effects, making them leads for further in vitro validation. These findings support the creation of a new siRNA-based treatment for HSV-1. By silencing important viral genes, this method could effectively reduce replication and reactivation, offering a promising alternative or complement to current antiviral therapies.



PD-DB-019: Development and Evaluation of Intranasal lactoferrinbased Duloxetine *In Situ* Nasal Gel for Targeting the Brain

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Background: Depression is a debilitating neurological condition affecting millions globally. Current treatment strategies, such as oral administration of Duloxetine, often suffer from poor bioavailability due to extensive first-pass metabolism and limited brain penetration. Intranasal drug delivery presents an advantageous route for direct nose-to-brain transport, bypassing systemic metabolism and enhancing therapeutic efficiency. Lactoferrin, a naturally occurring iron-binding glycoprotein, is gaining recognition for its role as a targeting ligand owing to its receptor-mediated endocytosis across the blood-brain barrier.

Aims & Objectives: The present study was designed to formulate and evaluate an intranasal in situ gel of Duloxetine using Lactoferrin as a targeting ligand to enhance brain delivery and therapeutic effectiveness in depression.

Methods: Duloxetine was characterized using melting point analysis, FTIR, and DSC techniques. In situ nasal gels were formulated using varying concentrations of Poloxamer 407 and HPMC K4M. A 3² factorial design was applied to optimize the formulation. The gels were evaluated for pH, viscosity, gelation temperature, drug content, mucoadhesive strength, in vitro release, ex vivo permeation, and isotonicity. Stability and cytotoxicity (RAW 264.7 cell line) studies were also conducted.

Results: All formulations displayed acceptable pH, clarity, and viscosity. The gelation temperature was in the desired physiological range (29–38°C), with formulation F3 showing optimal properties. Drug content ranged between 68.09–96.14%. In vitro and ex vivo studies demonstrated sustained drug release and effective mucosal permeation. The optimized batch exhibited good stability and was non-cytotoxic.

Conclusion: The developed Lactoferrin-based Duloxetine in situ nasal gel offers a novel, non-invasive platform for targeted brain delivery, overcoming limitations of conventional oral therapy. This formulation holds potential for improving the therapeutic management of depression.

Keywords: Duloxetine, Intranasal Gel, Lactoferrin, Nose-to-Brain Delivery, Depression, Mucoadhesion.



PD-DB-020: Design of a dual-compartment enteric-coated capsule to minimize capecitabine-PPI interaction and enhance therapeutic activity via albumin co-administration

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Background: Capecitabine, an oral prodrug of 5-fluorouracil (5-FU), is widely used in the treatment of advanced gastrointestinal cancers. Its bioavailability is pH-dependent, with optimal absorption occurring in the proximal small intestine. Proton pump inhibitors (ppis), frequently prescribed alongside chemotherapy for gastrointestinal protection, raise gastric pH and interfere with capecitabine dissolution and absorption, resulting in reduced efficacy. There is a critical need for a formulation strategy that can prevent this drug-drug interaction and improve therapeutic outcomes.

Aim and Objectives:

The aim of this study is to develop a novel **dual-compartment oral capsule** designed to:

1. Physically and functionally separate the release of capecitabine and PPI.
2. Protect capecitabine from premature gastric dissolution using enteric coating.
3. Enhance systemic and tumor-specific delivery by adjunct intravenous albumin co-administration.

Methods: A hard gelatin capsule was designed with two compartments: The **capsule body** contains **enteric-coated capecitabine granules or pellets**, using pH-sensitive polymers such as **Eudragit® L100** or **HPMCAS** (50–100 µm thickness), allowing drug release only at pH > 6.0 in the duodenum/jejunum. The **capsule head** is loaded with **immediate-release PPI granules** (e.g., omeprazole 20–40 mg), formulated for rapid disintegration in the stomach to achieve early acid suppression without interfering with capecitabine release. Additionally, **intravenous albumin** is proposed to be administered in combination to facilitate tumor targeting via SPARC-mediated uptake and the enhanced permeability and retention (EPR) effect. Capsule size 0 was selected based on dose volume and coating layer compatibility. In vitro dissolution, release kinetics, and pharmacokinetic modeling will be performed to simulate performance.

Conclusion: This novel dual-compartment enteric-coated formulation provides a rational and targeted approach to **eliminate the negative interaction** between capecitabine and ppis, restoring drug bioavailability and ensuring proper site-specific release. The inclusion of albumin co-administration is expected to enhance **tumor targeting, prolong circulation, and maximize therapeutic efficacy** with reduced systemic toxicity. This formulation approach holds significant potential for improving outcomes in patients with advanced gastrointestinal malignancies who require concurrent acid-suppressive therapy.

Keywords: Capecitabine, Proton Pump Inhibitor, Enteric Coating, Drug Interaction, Albumin Nanocarrier, Gastrointestinal Cancer, Dual-compartment Capsule, Bioavailability Enhancement, Targeted Drug Delivery



PD-DB-021: Design and Development of Enhanced Bioavailability Transdermal Patches for Carvedilol in Chronic Heart Failure Management

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Background: Carvedilol is a non-selective β -blocker commonly used for treating hypertension and other cardiovascular conditions. However, its oral administration poses several challenges such as rapid absorption, a short half-life of 7–10 hours, and high plasma protein binding, leading to fluctuating plasma levels and frequent dosing. These limitations reduce patient compliance and therapeutic effectiveness.

Aims & Objectives: This study aims to develop and evaluate transdermal patches of carvedilol to overcome the limitations of its oral route by enhancing bioavailability and ensuring sustained drug release. The objective is to formulate patches using various polymer combinations and assess their physical and in-vitro performance to identify the most effective formulation.

Methods: Transdermal patches were prepared using the solvent evaporation technique with different ratios of chitosan, Eudragit, and HPMC. Span 80 was used as a permeation enhancer, and glycerin served as a plasticizer. The formulated patches were evaluated for physical parameters including thickness, weight variation, drug content, flatness, tensile strength, folding endurance, moisture uptake, and moisture loss. In-vitro drug release studies were carried out over 12 hours to determine drug diffusion profiles.

Results: Patch thickness ranged from 0.524 ± 0.070 mm to 0.716 ± 0.045 mm, and weight varied between 0.092 ± 0.017 g and 0.166 ± 0.018 g. Drug content uniformity ranged from $78.9 \pm 0.010\%$ to $98.0 \pm 0.002\%$. Moisture uptake and loss were between $9.43 \pm 2.69\%$ to $26.7 \pm 8.17\%$ and $4.80 \pm 0.07\%$ to $22.82 \pm 1.60\%$, respectively. Folding endurance varied from 103 ± 3.6 to 384 ± 3.51 folds, and tensile strength from 0.3267 ± 0.0040 to 0.5450 ± 0.0010 kg/cm². In-vitro drug release ranged from $45.53 \pm 1.74\%$ (F8) to $82.58 \pm 1.52\%$ (F2) at 12 hours.

Conclusion: Formulation F2, containing chitosan, exhibited the best sustained release profile with $82.58 \pm 1.52\%$ drug release over 12 hours, suggesting its potential for effective transdermal delivery of carvedilol.

Keywords: Transdermal Patch, Controlled release, Bioavailability, *In-vitro*.



PD-DB-022: Intranasal in Situ Gelling Systems Of Resveratrol

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Background: Resveratrol, a polyphenolic compound known for its neuroprotective and antioxidant properties, suffers from low oral bioavailability due to rapid metabolism and poor gastrointestinal absorption. Intranasal delivery offers a direct route to the brain, bypassing the blood-brain barrier and hepatic first-pass metabolism. In situ gelling systems that transform from sol to gel at physiological conditions can enhance nasal retention and drug absorption.

Aims & Objectives: This study aimed to formulate and evaluate a thermosensitive in situ nasal gel of resveratrol using a combination of biocompatible polymers to improve drug stability, prolong residence time, and enhance brain targeting.

Methods: Six formulations (F1–F6) were developed using Poloxamer 407, Chitosan-CMC, and Gellan gum, dispersed in distilled water and cooled overnight at 4°C. Resveratrol and citric acid were added the next day, followed by pH adjustment to 6.4 using 0.1N NaOH. The prepared gels were stored at 4°C. Formulations were evaluated for clarity, pH, drug content, gelling temperature, gelling time, and physical appearance. FTIR analysis was conducted to check for drug-excipient interactions.

Results: Formulation F4 exhibited the most desirable profile with a gelling temperature of 34.1°C, gelling time of 42.6 seconds, and pH 6.4, suitable for nasal application. Drug content across formulations ranged from 85.2% to 94.3%. FTIR studies confirmed no significant interaction between resveratrol and polymers. The gel was clear in appearance and showed sustained drug release over 6–8 hours.

Conclusion: The developed in situ nasal gel system successfully enhanced resveratrol delivery by improving its solubility, stability, and nasal residence time. This platform holds promises for effective brain targeting and treatment of neurodegenerative disorders.

Keywords: Resveratrol, in situ gel, intranasal delivery, Poloxamer 407, neuroprotection, brain targeting, bioavailability.



PD-DB-023: Formulation and *In-Vitro* Evaluation of Transdermal Patch Containing Atorvastatin and Telmisartan for Combination Therapy

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Background: Hyperlipidaemia and hypertension represent two major modifiable risk factors for cardiovascular diseases, contributing significantly to atherosclerosis, myocardial infarction, and stroke. Current oral therapies, including atorvastatin (antihyperlipidemic) and telmisartan (antihypertensive), are limited by first-pass metabolism, gastrointestinal side effects, and poor patient compliance with daily dosing regimens.

Aims & Objectives: This study was aimed to develop a novel transdermal drug delivery system incorporating both atorvastatin and telmisartan to overcome the limitations of oral administration while ensuring sustained drug release and improved therapeutic efficacy in managing these comorbid conditions.

Methods: Twelve transdermal matrix patch formulations (F1-F12) were prepared using polymer blends of HPMC K15M, PVP K30, and Eudragit RS 100, along with plasticizers and penetration enhancers. The formulations were evaluated for physicochemical properties (thickness, tensile strength, folding endurance), moisture-related characteristics (uptake and loss), swelling index, in vitro drug release, and ex vivo permeation studies using pig skin.

Results: Formulation containing HPMC K15M (220 mg) and Eudragit RS 100 (180 mg), demonstrated the most favorable characteristics. The in vitro diffusion studies showed sustained release profiles with $42.78 \pm 1\%$ and $45.10 \pm 1\%$ for atorvastatin (D1) and telmisartan (D2), respectively, over 8 hours. The drug diffusion with ex vivo permeation was $35.14 \pm 1\%$ and $36.52 \pm 1\%$, respectively, for atorvastatin and telmisartan. The formulation exhibited excellent mechanical properties and stability, with drug release following Higuchi's kinetic model, indicating a diffusion-controlled mechanism.

Conclusion: The developed dual-drug transdermal patch presents a promising alternative to conventional oral therapy for concurrent hyperlipidaemia and hypertension management. The design offers sustained drug release, enhanced permeation, and potentially improved patient compliance, addressing key limitations of current treatment approaches.

Keywords: Atorvastatin, telmisartan, transdermal drug delivery, hyperlipidaemia, hypertension, sustained release, matrix patch, penetration enhancers



PD-DB-024: Design and Development of a Dual-drug loaded Nanostructured Lipid Carriers for Target Diabetic Wound Healing

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Background: Diabetic wounds are characterized by impaired healing due to dysregulation of molecular pathways involving HIF-1 α , VEGF and Wnt/ β -Catenin. Stabilization of HIF-1 α by inhibiting its degradation via the VHL-mediated ubiquitin-proteasome pathway is a promising therapeutic strategy. Synephrine, identified through *in-silico* methods as a potential VHL:HIF-1 α PPI inhibitor, alongside zinc oxide (zno), known for its antimicrobial and regenerative properties, was selected for Nano formulation.

Aims & Objectives: To formulate, optimize & characterize Synephrine and zno loaded Nanostructured Lipid Carrier (NLC) using Box-Behnken design for enhance diabetic wound healing efficacy

Methods: Nlc was prepared by micro emulsion method & optimized with Box-Behnken design (3 factors, 3 levels: -1, 0, +1) was employed to optimize NLC formulation. The factors included lipid ratio (20%, 30%, 40%), surfactant concentration (0.5%, 0.75%, 1%), and homogenization speed (4000, 6000, 8000 rpm). Responses measured were particle size, zeta potential, and polydispersity index. The external morphology of the NLC was characterized by SEM and TEM. Further the formulation was char for entrapment efficacy, crystallinity (DSC) & *in-vitro* release kinetics

Results: The optimized NLC have the particle size 113 nm, ZP 51 mv & PDI 21.4% and Characterization confirms the shape & size of the NLC. 82% of Synephrine drug was encapsulated in the NLC. The encapsulated Synephrine is expected to bind to VHL, inhibiting the HIF-1 α degradation pathway. Zno further contributes by promoting tissue regeneration, reducing oxidative stress, and providing antimicrobial activity, collectively enhancing diabetic wound healing.

Conclusion: A dual drug loaded NLC incorporating Synephrine and zno was successfully optimized and characterized, representing a novel and targeted nanotherapeutic approach for diabetic wound healing.

Keywords: Diabetic wound healing, HIF-1 α , VHL, Zinc oxide, NLC, Box-Behnken design.



PD-DB-025: Formulation and Characterization of Risperidone loaded lipid Nanocapsules for enhanced solubility

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Background: Schizophrenia is a debilitating and chronic psychiatric illness that severely compromises the quality of life of patients. The clinical efficacy of risperidone is compromised by its low oral bioavailability and short half-life.

Aims & Objectives: The current research investigates the application of lipid nanocapsules (Incs) as a new delivery platform to improve the solubility and bioavailability of risperidone.

Methods: Preformulation investigations were performed to check the compatibility of risperidone with the excipients chosen. Incs were prepared by the PIT method and optimized by a Design of Experiments (doe) strategy. The optimized Risperidone Incs were characterized and evaluated by Size, PDI, Zeta potential, %EE, and in vitro dissolution study.

Results: The optimized formulation had a particle size of 256.8 nm, polydispersity index (PDI) of 0.309, zeta potential of -48.1 mv, and encapsulation efficiency of 77.62%. In vitro release profiles showed the sustained release pattern, with about 94% cumulative drug release within 24 hours.

Conclusion: These results indicate the potential of Incs to improve the solubility, stability, and bioavailability of risperidone, thus offering a promising way to enhance its therapeutic efficacy in the treatment of schizophrenia.

Keywords: Solubility, Lipid Nano capsules, Schizophrenia, Risperidone.



PD-DB-026: Quercetin Nanoemulsion Ameliorates Key Hallmarks of Lung Cancer

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Background: Lung cancer remains one of the most lethal malignancies worldwide, with limited therapeutic outcomes due to drug resistance, off-target toxicity, and suboptimal drug delivery. Quercetin, a naturally occurring flavonoid, has demonstrated potent anti-inflammatory and anti-cancer properties. However, its clinical potential is restricted by poor aqueous solubility, low bioavailability, and rapid metabolic degradation. Nanoemulsion-based drug delivery systems offer a promising strategy to overcome these limitations and enhance therapeutic efficacy.

Aims & Objectives: This study aims to evaluate and compare the anti-cancer efficacy of quercetin nanoemulsion (QNE) and quercetin pure drug (QPD) in A549 human lung adenocarcinoma cells, while also determining their safety profile on healthy cells.

Methods: QNE and QPD were tested at various concentrations on both cancerous and non-cancerous cell lines to determine cytocompatibility. Functional assays including MTT-based cell proliferation, wound healing migration and colony formation assays were conducted. The expression of key oncogenic genes and proteins involved in angiogenesis, metastasis and cell cycle regulation was assessed. Furthermore, *in silico* approaches including network pharmacology and molecular docking were performed to elucidate quercetin's molecular targets and validate mechanistic correlations.

Results: QNE showed significantly greater inhibition of A549 cell proliferation, migration, and colony formation compared to QPD, while exhibiting minimal cytotoxicity in healthy cells. Molecular studies confirmed substantial downregulation of cancer-promoting genes and proteins following QNE treatment. Computational analyses further supported these findings, revealing strong binding affinities of quercetin with multiple cancer-related molecular targets.

Conclusion: The quercetin nanoemulsion exhibited enhanced anti-cancer activity over its pure drug form, likely due to improved solubility, stability, and cellular uptake. These results



highlight QNE's potential as a novel and effective therapeutic strategy for lung cancer. Further *in vivo* validation is essential to support its clinical translation.

Keywords: Quercetin; Nanoemulsion; Lung Cancer; Migration; Proliferation



PD-DB-027: Design, optimization, and characterization of Melatonin loaded Solid lipid nanoparticles for enhanced treatment of sleep disorders

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Background: Melatonin (MLT) belongs to BCS class II and shows poor bioavailability when administered orally because of its low solubility and short half-life. It rapidly undergoes first-pass metabolism, which poses significant challenges in its use in treating sleep disorders.

Aims & Objectives: The objective of the study was to develop and evaluate Melatonin-loaded Solid Lipid Nanoparticles (slns) to improve MLT's bioavailability and therapeutic efficacy in treating sleep disorders.

Methods: The MLT-slans were optimized using the Box-Behnken Design (BBD) and developed by hot homogenization followed by ultrasonication. All formulations were characterized for particle size, zeta potential, entrapment efficiency, and percentage cumulative drug release (CDR).

Results: FTIR results revealed no major interaction between the selected drug Melatonin, lipid (Tristearin), and surfactants (soya lecithin and tween 80). The optimized formulation (without charge modifier) had a particle size of 40.15 nm, with a PDI of 0.467 and a ZP of -16.50 mv, drug content of 97.54 ± 0.87 % and entrapment efficiency of 86.23 ± 0.32 %. Stearyl amine was added as a charge modifier, increasing particle size to 55.06 nm and shifting the ZP to +17.5 mv. It shows an entrapment efficiency of 87.65 ± 2.48 % and drug content of 97.54 ± 0.346 %. SEM images depicted that every particle was a distinct entity with a smooth surface and a mixture of spherical and asymmetric. The CDR was 92.06 and 98.46 % for formulations without and with stearyl amine, respectively, with a biphasic release pattern (immediate and sustained release). Both formulations followed zero-order release kinetics (R^2 values 0.9858 and 0.978).

Conclusion: Melatonin was successfully incorporated into tristearin-based solid lipid nanoparticles and produced stable slns. The doe-suggested optimal formulation was proved for particle size, entrapment efficiency, and drug release profile.

Keywords: Solid lipid nanoparticles, Melatonin, Box Behnken design, sleep disorders, stearyl amine.



PD-DB-028: Development of Fast-Dissolving Film of Tramadol Hydrochloride And Evaluation of Properties Using Natural and Synthetic Polymer

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Background: Tramadol hydrochloride, a serotonin-norepinephrine reuptake inhibitor belongs to BCS class I category of drug. It is frequently used to treat moderate to severe pain, especially pain following surgery. Fast dissolving films offer a practical way to administer drugs quickly, particularly where a rapid commencement of action is preferred.

Aim and Objective: The present work was designed with an aim to develop fast-dissolving films of tramadol hydrochloride and evaluate its physicochemical and mechanical properties.

Methods: Hydroxypropyl methylcellulose (HPMC E15) was used as a polymer both alone and in conjunction with sodium alginate to create fast-dissolving films. The polymeric films were prepared using polyethylene glycol 400 as plasticizer. Thickness, weight variation, surface pH, folding endurance, moisture content, Fourier-transform infrared spectroscopy (FTIR), in vitro disintegration time, and in vitro drug dissolution were among the mechanical and physicochemical parameters that were assessed for the films.

Results: The mechanical and physicochemical characteristics of every formulation were satisfactory. F7 had a mean disintegration time of 34 seconds and the maximum drug release (97.67%) within 30 minutes among the formulations. There were no discernible changes in factors like stability, drug content, or physical appearance.

Conclusion: Tramadol hydrochloride film can be made by using the solvent casting method with HPMC E15 and sodium alginate as polymers. The films provide rapid drug release and may be a suitable alternative dosage form for immediate pain relief.

Keywords: Tramadol hydrochloride, BCS Class I, fast-dissolving film, solvent casting, HPMC E15, sodium alginate.



PD-DB-029: Comparative studies of branded and generic tablets of various brands of clarithromycin

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AIM-The present study focuses on the comparative evaluation of generic and branded formulations of Clarithromycin 250 mg tablets to assess their pharmaceutical equivalence and ensure compliance with pharmacopeial standards. Clarithromycin, a macrolide antibiotic, is widely used for treating bacterial infections, and its consistent quality is essential to ensure therapeutic efficacy. With the increasing availability of generic versions, there is a critical need to assess whether these alternatives meet the same quality benchmarks as branded products.

METHODS- This study involved the systematic analysis of multiple physical and chemical quality control parameters. Six key in vitro tests were performed: weight variation, friability, disintegration, thickness, diameter, hardness, and dissolution testing. Weight variation and thickness were measured to assess uniformity and consistency in tablet formulation, while hardness and friability tests evaluated mechanical strength and resistance to physical stress during handling. Disintegration time was recorded to determine the tablet's ability to break down in the gastrointestinal environment, a prerequisite for drug release and absorption. The dissolution test was conducted using USP Apparatus II (paddle method) in 0.1 N HCl to evaluate the drug release profile, a crucial indicator of bioavailability.

RESULTS- Demonstration of notable variations between the generic and branded tablets in certain parameters, although all samples complied with pharmacopeial limits. Branded tablets generally showed superior physical characteristics, such as higher hardness and lower friability, contributing to better handling and storage stability. However, dissolution profiles of the generic tablets were found to be comparable, suggesting that they could provide equivalent therapeutic outcomes.

CONCLUSION- Minor differences were observed in physical parameters, the overall results indicate that selected generic Clarithromycin tablets are pharmaceutically equivalent to the branded product. This supports the safe and effective substitution of branded drugs with cost-effective generic alternatives, provided they meet all regulatory quality standards.



PD-DB-030: Formulation and Evaluation of Ocimum Basilicum extract loaded Pain Reliever Balm

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In today's fast-paced world, tension headaches have become almost a daily companion for many. They're often triggered by stress, poor posture, or long hours of screen time. While pills offer systemic relief, pain balms provide a targeted, fast-acting solution right where it hurts. Basil (*Ocimum basilicum*) is an important crop recognized for its essential oils, polyphenols, phenolics, flavonoids, and phenolic acids. This annual plant originates from tropical regions and belongs to the mint family. The purpose of this study was to draw attention to the value of phytochemical-based formulations in the management of pain and inflammation from various causes while avoiding the potential negative effects of conventional therapies. Our formulation relies on the use of an *Ocimum basilicum* extract, which has been shown to have anti-inflammatory, analgesic, and antioxidant properties in vitro. The balm is crafted through a careful process: petroleum jelly and beeswax are melted and combined to create the base, enhanced with camphor for cooling relief, menthol for added comfort, and BHT (Butylated hydroxy toluene) for stability. The sweet basil extract is dissolved in ethanol and mixed into the base, which once cooled, transforms into a smooth, semi-solid ointment. Evaluation of a pain-relieving balm included organoleptic checks, pH, spreadability, viscosity, and stability. Safety was assessed via skin irritation and microbial load tests. Active ingredient content and uniformity ensured efficacy. Optional studies included in-vitro permeation and therapeutic testing to validate pain relief and anti-inflammatory properties of the formulation. The evaluation of the pain-relieving balm demonstrates its potential as an effective formulation for pain relief and anti-inflammatory benefits.

Keywords: *Ocimum basilicum*, pain reliever, semi-solid ointment, analgesic
Anti-inflammatory



PD-DB-031: Development of Novel Co-Processed Excipients for the Design and Evaluation of Fast Dissolving Meclizine Hydrochloride Tablets

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Background: Fast-dissolving tablets (fdts) require excipients with excellent flowability and compressibility. Co-processing through spray drying is an effective method to enhance these properties compared to physical mixtures.

Aims & Objectives: This study aimed to develop co-processed excipients for fdts using spray drying. The objectives included:

- Preparing co-processed excipients in various ratios of MCC, sodium starch glycolate, mannitol, and Aerosil
- Evaluating flow and compressibility properties (Carr's index, Hausner's ratio, angle of repose)
- Formulating Meclizine Hydrochloride fdts using the co-processed excipients
- Comparing the performance of tablets made with co-processed and physical mixtures
- Assessing drug-excipient compatibility and formulation stability.

Methods: Co-processed excipients were prepared using:

- MCC: Sodium starch glycolate: Aerosil (90:8:2, 90:6:4, 90:5:5)
- Mannitol: MCC: Aerosil (80:18:2, 80:16:4, 80:14:6)

These were evaluated for flow properties and used in FDT formulations of Meclizine Hydrochloride. Dispersion time, stability, and IR spectroscopy were studied.

Results: Co-processed excipients showed improved flow (angle of repose $<30^\circ$), Carr's index (10–14.81%), and Hausner's ratio (1.10–1.16). Fdts with MCSGA (90:8:2) and MMCA (80:18:2) had faster dispersion times (24.26 s and 32.37 s) than physical mixtures (56.15 s and 62.9 s). No significant changes were seen in stability or IR studies.

Conclusion: Co-processed excipients significantly enhanced the flow, compressibility, and dissolution performance of Meclizine Hydrochloride fdts compared to physical mixtures.

Keywords: Co-processed excipients, Spray drying, Fast dissolving tablets, Meclizine Hydrochloride.



PD-DB-032: Formulation and *in-vitro* evaluation of ufasomal topical gel containing antifungal agent

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Background: Fungal skin infections are one of the most common dermatological concerns nowadays. Ketoconazole is an imidazole antifungal agent used in the prevention and treatment of a variety of fungal infections.

Aims & Objectives: The study aimed to develop and evaluate oleic acid vesicles loaded with antifungal agent for the topical treatment of fungal infections.

Methods: Ketoconazole-loaded ufasomes were prepared by the thin film hydration method using varied concentrations of oleic acid and Span 80. All formulations were characterized for particle size, zeta potential, entrapment efficiency, FTIR, and Scanning Electron Microscope. Then, ufasomes were incorporated into a Carbopol gel base and evaluated for drug content, pH, Spreadability, viscosity, *in-vitro* drug diffusion, and short-term stability study.

Results: The developed Ketoconazole-loaded ufasomes show entrapment efficiency, ranging from 50% to 75%, with particle sizes ranging between 160 nm and 300 nm, and exhibited a zeta potential of -26.9 mv. SEM images show that formulated ketoconazole-loaded ufasomes were well-identified as spherical vesicles with uniform size distribution. The Optimized formulations show an 83.4% cumulative drug release for 16 hr with Korsmeyer-Peppas drug release pattern. Formulated ufasomal gel shows smooth texture with optimum pH, viscosity, and spreadability. No significant changes in pH, drug content, or cumulative percentage drug release were found in the stability data.

Conclusion: Ketoconazole was successfully incorporated into oleic acid-based ufasomes. The Ufasomal gel formulation of Ketoconazole can be used for the treatment of fungal infections with improved bioavailability.

Keywords: Ketoconazole, ufasomal gel, fungal infections, oleic acid.



PD-DB-033: Development and characterization of plumbagin-loaded liquid crystalline nanoparticles for the targeted therapy of triple negative breast cancer.

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Background: Triple-negative breast cancer (TNBC) is a highly aggressive form lacking estrogen, progesterone, and HER2 receptors, rendering current therapies largely ineffective and prone to multidrug resistance. Plumbagin, a phytochemical from *Plumbago zeylanica*, has demonstrated potent anticancer activity, but suffers from poor bioavailability and systemic toxicity.

Aim & Objectives: To develop and evaluate a safe and effective plumbagin-loaded liquid crystalline nanoparticle (LCNP) delivery system for targeted therapy of TNBC, aiming to improve drug stability, bioavailability, and cytotoxicity against TNBC cells.

Methods: Plumbagin-loaded lcnps were prepared using the ultrasonication method and optimized using a Box-Behnken design. The formulation was characterized for particle size, PDI, zeta potential, drug entrapment efficiency, and morphology. In vitro drug release, stability studies, and cytotoxicity assays on MDA-MB-231 cell lines were also conducted.

Results: Optimized lcnps had a particle size of 224 d.nm, PDI of 0.129, and zeta potential of +22.4 mv. Entrapment efficiency reached 82.4%, with 97% sustained drug release over 96 hours. Cytotoxicity studies revealed IC₅₀ values of 25.93 µg and 12.75 µg after 24 and 48 hours, respectively, indicating potent anti-TNBC activity.

Conclusion: Plumbagin-loaded lcnps demonstrated excellent stability, sustained drug release, and enhanced cytotoxicity against TNBC cells, offering a promising nanocarrier system for targeted breast cancer therapy.

Keywords: Triple-negative breast cancer, Liquid crystalline nanoparticles, Plumbagin, Targeted drug delivery, In vitro cytotoxicity, Nanotechnology



PD-DB-034: Formulation & Evaluation of Levofloxacin Nanosponge Hydrogel

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Background: Levofloxacin is a broad-spectrum antibiotic used for treating skin infections, but its conventional topical delivery poses challenges in sustained release. Nanosponges offer a promising solution by enhancing drug stability and providing controlled release. Incorporating Levofloxacin into a nanosponge-based hydrogel enables prolonged antimicrobial activity and improved therapeutic efficacy.

Materials And Methods: Hydrogels are polymeric material that exhibits the ability to swell and retain a significant fraction of water within its structure but will not dissolve in water. In the current study, Levofloxacin loaded nanosponges (NS) were fabricated by solvent emulsion evaporation method, using different concentration of ethyl cellulose (EC) as a rate retarding polymer. Prepared NS were characterized for particle size (PS), polydispersity index (PDI), zeta potential (ZP), entrapment efficiency (EE), drug content and percentage yield. It was further evaluated for physicochemical characterizations; FTIR, DSC and SEM

Results and Discussion: The results of percentage yield, particle size (PS), polydispersity index (PDI), zeta potential (ZP) and entrapment efficiency (EE) showed the satisfactory results and drug content found within the limits. SEM result shows nanosponges were porous with a smooth surface morphology and. The formulated NS was incorporated into the (1%, w/w or w/v) Carbopol gel. NS based hydrogel was then evaluated for viscosity, Spreadability, pH, in-vitro release, antibacterial. The NSH3 formulation showed the drug release of 70.1% respectively at the end of sixth hour with Higuchi model following anomalous Fickian drug release. Increase of drug release was observed as a function of drug: polymer ratio.

Conclusion: The developed Levofloxacin nanosponge hydrogel system presents a promising approach for improving the therapeutic efficacy and patient compliance in the treatment of bacterial infections through localized and sustained drug delivery.

Keywords: Nanosponge Hydrogel, Bacterial infections, sustained release.



PD-DB-035: Formulation and Characterization of Biogenic Silver Nanoparticle-Loaded Hydrogel Using Latex of *Calotropis Gigantea* For Topical Wound Healing

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Background: The current study focusses on creating and characterising a hydrogel filled with silver nanoparticles utilising *Calotropis gigantea* latex for topical wound healing and anti-inflammatory purposes. Silver nanoparticles (agnps) were synthesized using the latex extract through a biogenic approach and it is characterized using UV-Vis spectroscopy, FTIR, SEM, TEM, XRD, and DSC, the result confirmed that the stable, agnps with nanoscale shape developed. The synthesized agnps were incorporated into a hydrogel formulation, and it was evaluated for pH, Spreadability, viscosity, The hydrogel is subjected to biological and physicochemical assessments such as in vitro diffusion studies, and antibacterial activities. The formulation exhibited stable pH for topical application, excellent Spreadability & viscosity, the hydrogel also demonstrated sustained drug release. Based on the documented anti-inflammatory and wound healing properties of both *C. Gigantea* and silver nanoparticles the developed biogenic agnp-loaded hydrogel bears potential as safe, stable and effective topical formulation

Aims & Objectives: To develop and evaluate a silver nanoparticle loaded hydrogel using *C.gigantea* latex for potential wound healing and anti-inflammatory activity.

Objectives:

- To extract latex from *Calotropis gigantea* To characterize the synthesized silver nanoparticles
- To formulate a bioactive hydrogel loaded with synthesized agnps
- To evaluate the physicochemical properties of the hydrogel
- To assess the in vitro drug release profile of hydrogel
- To investigate the biological activities of hydrogel
- To determine the hydrogel's potential as a safe, stable, and effective wound healing

Methods: The hydrogel formulation has been developed with carbopol as the gelling agent, polyethylene glycol (PEG) as a humectant, triethanolamine for pH correction and gel formation, and sodium benzoate as a preservative. Silver nanoparticles synthesised from *Calotropis gigantea* latex were mixed into this base to create a stable, bioactive hydrogel. The produced formulation was subjected to in vitro diffusion tests to assess drug release behaviour. The study found that the active component was released most effectively around 150 minutes, showing sustained and regulated distribution from the hydrogel matrix. In addition, the hydrogel was tested for antibacterial activity against specific harmful microorganisms. The compound showed significant antibacterial activity, indicating its potential for wound healing applications

Result: The silver nanoparticles has been prepared showed acceptable range of UV-V spectroscopy. From in vitro release of study, it was observed that all formulations extended the release to up to 6 hours.



Conclusion: This formulation can be used to reduce the infection caused by wound, will have more acceptance from the patient and give rapid onset of action.

Key words: Calotropis gigantea (C. Gigantea), Silver Nanoparticle (agnps), Hydrogel, Wound healing, Anti-inflammatory, Anti-microbial activity.

PD-DB-036: Development of *In-situ* gel formulation for local treatment of periodontitis

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Background: Periodontitis is a chronic gum infection that harms the soft tissues and bone around the teeth. Secnidazole is a second-generation antimicrobial drug belonging to nitroimidazole class. It targets the various anaerobic gram-positive and gram-negative bacteria. *In-situ* gel formulation provides localized action with sustained release.

Aims & Objectives: The aim of the study was to develop a syringeable *in-situ* gelling formulation of Secnidazole for enhanced local treatment of periodontitis, by providing sustained drug release.

Methods: *In-situ* gel formulation was prepared by cold method by dissolving polymer in a cold phosphate buffer (ph 6.8) under constant stirring and it was refrigerated until further use. Six formulations were prepared with varying concentration of Poloxamer-407 (20-22% w/v), poloxamer-188 (1% w/v), HPMC E5 (0.5% W/V) and drug (0.5%-1.5% w/v). These formulations were evaluated for syringeability, gelation time, gelation temperature, ph, and in-vitro antibacterial activity.

Results: The results demonstrated that all formulations were easily syringeable using a 21-gauge needle at cold temperatures. The gelation temperature ranged between $37.5 \pm 1^\circ\text{C}$ and $39.2 \pm 0.5^\circ\text{C}$, while the ph values ranged from 7.03 ± 0.05 to 7.46 ± 0.05 . The drug release profiles indicated sustained release over 8 hours, with formulations releasing $43 \pm 0.5\%$ to $56 \pm 0.4\%$ of the drug during this period.

Conclusion: Prepared *in-situ* gelling system provides a newer dimension for the effective management of periodontitis. The preparation of formulation is simple and reproducible. This system provides localized effect increasing the therapeutic effect.

Keywords: Secnidazole, *in-situ* gel, thermoreversible polymers, controlled drug release, periodontitis, antibacterial activity.



PD-DB-037: Formulation and Evaluation of Jackfruit Mucilage-Based Sustained Release Transdermal Patches of Clopidogrel Bisulphate

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Background: Clopidogrel bisulphate is an antiplatelet used to reduce the risk of myocardial infarction, stroke and cardiovascular and cerebrovascular disease. It is having low oral bioavailability (50%) and significant first pass metabolism. To overcome the limitation of oral dosage form, transdermal drug delivery offers a non-invasive and sustained release system. Natural polymers like jackfruit mucilage have gained interest due to their bio-compatibility and biodegradability.

Aims & Objectives: This study aimed to formulate and evaluate sustained-release transdermal patches of Clopidogrel bisulphate using jackfruit mucilage as a natural polymeric matrix and to evaluate the patches for different physicochemical and mechanical parameters.

Methods: Patches were prepared by solvent casting with varying polymer-drug ratios. The natural polymer (*Artocarpus heterophyllus*) Jackfruit mucilage and synthetic polymer polyvinyl alcohol with different ratios from formulations (F1-F7) along with polyethylene glycol was used as plasticizer. The formulated patches were evaluated for physicochemical parameters such as thickness, folding endurance, moisture content, drug content, and in vitro drug release.

Results: Among all the formulations, F4 showed sustained release at 54.05% in 8 hours. The drug release kinetics followed first order release with non-fickian diffusion mechanism. Other formulations also exhibited satisfactory physicochemical properties and controlled release patterns, supporting the potential of jackfruit mucilage as an effective matrix former.

Conclusion: The study concludes that jackfruit mucilage-based transdermal patches of Clopidogrel bisulphate is promising for sustained drug delivery and may serve as a natural alternative to synthetic polymers in controlled release formulations.

Keywords: Transdermal drug delivery system, Clopidogrel bisulphate, Jackfruit mucilage, Sustained release, Natural polymer.



PD-DB-038: ph-Responsive Polymeric Nanoparticles for Targeting Ovarian Cancer: Design, Optimization, And Development.

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Background: Ovarian cancer's late diagnosis, intricate molecular makeup, and resistance to traditional treatments make it one of the deadliest gynecological cancers. The PARP inhibitor olaparib, which works well against cancers with BRCA mutations, has low permeability and solubility. This work investigates how to improve the delivery of olaparib using ph-sensitive silk fibroin nanoparticles with surface modification by folic acid. Reducing systemic toxicity and increasing efficacy are achieved by targeting ovarian cancer cells that overexpress CD44.

Aims & Objectives: ph-sensitive nanoparticles loaded with olaparib were developed for the targeted treatment of ovarian cancer. Conjugation of folic acid enhances solubility, absorption, and selectivity for cells that express CD44. The formulation's physicochemical characteristics, therapeutic effectiveness, and cellular uptake were assessed.

Methods: Nanoprecipitation was used to formulate the nanoparticles, and Design Expert 13's full factorial design was used for process and product optimization. DLS examined the physicochemical characteristics (particle size, PDI, and zeta potential), while TEM verified the morphology. Additional characterization methods included ph-dependent in vitro drug release, DSC, and FTIR. Cellular uptake was measured using ovarian cancer cell lines, and biodistribution was examined in animals.

Results: Optimized formulation showed a zeta potential of -23 mv, a PDI of 0.1673, and a particle size of 183 nm. TEM verified particles less than 150 nm. Following ph 7.4 (60.53%) and ph 6.8 (50.72%), drug release peaked at ph 5.5 (71.61%). Biodistribution profiles suggested better tissue accumulation. Compared to their uncoated counterparts, coated nanoparticles demonstrated noticeably greater cellular absorption.

Conclusion: With improved solubility, cellular absorption, and therapeutic potential, the established ph-sensitive silk fibroin nanoparticles surface modified by Folic acid present a potentially targeted drug delivery platform for Olaparib. This approach opens the door for ovarian cancer with a BRCA mutation to be treated precisely.

Keywords: ph sensitive polymer, Olaparib, Silk fibroin, Ovarian cancer, Targeted delivery.



PD-DB-039: Metal oxide nanocomposite for topical drug delivery for the antimicrobial activity of syzigium samarangense extract

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Background: Topical drug delivery systems have gained importance due to their ability to provide localized therapeutic effects with minimal systemic side effects. In line with green chemistry principles, plant-mediated synthesis of nanoparticles presents a sustainable alternative to conventional chemical methods. The leaves of *Syzygium samarangense* are known to contain phytoconstituents that can aid in the eco-friendly synthesis of metal oxide nanocomposites.

Aims & Objectives:

- To develop a sustainable and eco-friendly method for synthesizing zirconium oxide (ZrO_2) nanoparticles using *Syzygium samarangense* leaf extract.
- To formulate a topical gel incorporating the synthesized ZrO_2 nanoparticles for potential cutaneous applications.
- To characterize the synthesized nanoparticles using various analytical techniques.
- To evaluate the suitability of the developed nanocomposite gel for topical drug delivery.

Methods: Phytoconstituents were extracted from *S. Samarangense* leaves and used as a reducing and stabilizing agent in the green synthesis of ZrO_2 nanoparticles. The nanoparticles were then incorporated into a carbopol-based topical gel. Characterization was performed using Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-ray (EDX) analysis, and Scanning Electron Microscopy (SEM) to evaluate functional groups, elemental composition, and morphological features.

Results: The SEM images confirmed the nanoscale morphology of the synthesized particles, while EDX analysis verified the presence of zirconium and oxygen, affirming the formation of ZrO_2 . FTIR spectra indicated the participation of phytochemicals in the reduction and stabilization process. The formulation of the gel was smooth and homogeneous, suggesting good dispersion and compatibility of the nanoparticles within the gel matrix. It also shown the antimicrobial activity of 9mm against *Pseudomonas aeruginosa*.

Conclusion: The study successfully demonstrated a green synthesis approach for preparing ZrO_2 nanoparticles using *Syzygium samarangense* leaf extract. The integration of these nanoparticles into a topical gel matrix represents a promising strategy for sustainable and effective cutaneous drug delivery applications.

Keywords: *Syzygium samarangense*, zirconium oxide nanoparticles, green synthesis



PD-DB-040: Development and Evaluation of Pectin-Based Herbal Periodontal Films Containing Papain and Cinnamon Oil for the Treatment of Periodontitis

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Periodontitis is a chronic inflammatory disease that affects the supporting structures of teeth, leading to tissue destruction and potential tooth loss. The current study aimed to develop a localized, herbal-based drug delivery system to manage periodontitis using pectin as a natural polymer matrix. Papain, known for its anti-inflammatory and wound-healing properties, and cinnamon oil, possessing antimicrobial and analgesic activity, were selected as the active ingredients. The films were prepared using the solvent casting method and optimized using Design-Expert® software for mechanical and physicochemical parameters. Comprehensive evaluations including Fourier Transform Infrared Spectroscopy (FTIR), tensile strength, drug content, in vitro release, and permeation studies were conducted. The formulation demonstrated sustained release profiles, efficient mucosal permeation, and significant antibacterial activity against *S. Aureus* and *E. Coli*. Furthermore, cell-line studies using MTT and crystal violet assays confirmed the biocompatibility and safety of the films, while TLR-4 assay indicated anti-inflammatory effects. Stability testing over 60 days revealed the films retained physical integrity and therapeutic efficacy. The results support the feasibility of pectin-based films as an effective, biocompatible, and patient-friendly approach for localized periodontitis therapy, leveraging herbal bio-actives to reduce inflammation and bacterial load while enhancing healing.

Keywords: Periodontitis, Papain, Cinnamon oil, Herbal periodontal film, Mucoadhesive film, Antibacterial, Anti-inflammatory.



PD-DB-041: Design and formulation of mucoadhesive mouth paints

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Background: Oral candidiasis is a common fungal infection, especially in immunocompromised patients, including those with AIDS or undergoing immunosuppressive therapy. Prolonged retention of the antifungal drug at the site of infection is crucial for effective treatment. Mucoadhesive formulations can enhance drug residence time and efficacy.

Aims & Objectives: The aim was to develop oral mucoadhesive mouth paint formulations containing fluconazole for prolonged antifungal activity.

The objectives were:

- To formulate 1% fluconazole mouth paints using various mucoadhesive polymers
- To evaluate the physicochemical and mucoadhesive properties
- To study in vitro drug release, stability, antifungal activity, and mucosal safety

Methods: Formulations were prepared using hydrophilic polymers such as HPMC, HEC, and nacmc, along with glycerol and sodium citrate. Evaluations included pH, drug content, rheology, spreadability, mucoadhesive strength, and IR spectroscopy. In vitro drug release was studied at pH 6.4 using a cellophane membrane. Stability testing was done at room temperature, $8 \pm 1^\circ\text{C}$, and $45 \pm 2^\circ\text{C}$ with $75 \pm 5\%$ RH for 3 months. Antifungal activity against *Candida albicans* was assessed using the agar cup-plate method. Mucosal irritancy tests were performed on rabbits, guinea pigs, and human volunteers.

Results: All formulations were stable under different conditions. Nacmc-based formulations exhibited superior mucoadhesive strength, spreadability, and larger zones of inhibition. No mucosal irritation or adverse reactions were observed in animals or human volunteers.

Conclusion: Mucoadhesive mouth paints of fluconazole, especially those with nacmc, demonstrated effective antifungal activity, good retention, stability, and safety, making them suitable for the treatment of oral candidiasis.

Keywords: Fluconazole, Mucoadhesive mouth paint, Oral candidiasis, Antifungal activity, In vitro release.



PD-DB-042: Development and Evaluation of Rizatriptan Benzoate Hybrid Nanoemulsion loaded *in-situ* nasal gel for Migraine

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Background: Migraine is a disabling neurological condition, affecting millions globally, particularly women. Rizatriptan benzoate, a potent 5-HT_{1B/1D} receptor agonist, has limited oral bioavailability due to high first-pass metabolism. Intranasal delivery offers a direct nose-to-brain route, avoiding hepatic metabolism and allowing rapid therapeutic onset.

Aim & Objectives: The aim of this study is to develop and evaluate a hybrid nano emulsion based *in-situ* nasal gel of Rizatriptan benzoate using Poloxamer 407 and sodium alginate for effective brain targeting and sustained migraine relief.

Methods: Nanoemulsion of Rizatriptan benzoate was prepared using the ultrasonication technique and optimized based on droplet size, zeta potential, polydispersity index, and drug entrapment efficiency. The optimized nano emulsion was incorporated into a temperature-sensitive *in-situ* gel using Poloxamer 407, and mucoadhesive sodium alginate was included to improve nasal retention and release control. The gel was evaluated for clarity, pH, gelation temperature, viscosity, gel strength, and *in-vitro* diffusion profile.

Results: The hybrid nano emulsion exhibited uniform nanodroplet size (<200 nm), stable zeta potential, and high drug entrapment efficiency. The *in-situ* gel formulation gelled at nasal cavity temperature (~32–34°C), showed suitable rheological properties, and achieved sustained drug release with enhanced nasal residence time due to the presence of sodium alginate.

Conclusion: The developed hybrid nanoemulsion-loaded thermoresponsive *in-situ* nasal gel provides a promising platform for nose-to-brain delivery of Rizatriptan benzoate. It effectively overcomes oral bioavailability issues, ensures rapid onset of action, and offers sustained migraine relief with improved patient compliance.

Keywords: Rizatriptan benzoate, Hybrid nanoemulsion, *In-situ* nasal gel, Nose-to-brain delivery.



PD-DB-043: Formulation and Evaluation of Vonoprazan Fumarate-Loaded Nanostructured Lipid Carriers for Gastroesophageal Reflux Disease

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Background: Gastroesophageal reflux disease (GERD) is a chronic condition characterized by the backflow of gastric contents into the esophagus, leading to symptoms like heartburn and acid regurgitation. Vonoprazan fumarate, a potassium-competitive acid blocker (P-CAB), offers superior acid suppression compared to traditional proton pump inhibitors but is limited by poor water solubility and low oral bioavailability.

Aim & Objectives: The aim of this study is to formulate and evaluate Vonoprazan fumarate-loaded nanostructured lipid carriers (nlcs) to enhance its solubility, bioavailability, and therapeutic efficacy for effective management of GERD.

Methods: Preformulation studies including solubility analysis, melting point determination, UV and FTIR spectroscopy were conducted to characterize the drug. Nlcs were prepared using a homogenization followed by ultrasonication method. The formulations were characterized for particle size (DLS), zeta potential, drug entrapment efficiency (UV spectroscopy), surface morphology (SEM/TEM), and *in-vitro* drug release.

Results: The optimized NLC formulation exhibited nanometric particle size, favorable zeta potential indicating stability, and high entrapment efficiency. The *in-vitro* release studies demonstrated a sustained drug release profile, confirming the suitability of the nlcs for controlled delivery. FTIR confirmed drug-excipient compatibility.

Conclusion: The developed Vonoprazan fumarate-loaded nlcs showed improved physicochemical properties and release characteristics, offering a promising strategy to overcome the drug's solubility and bioavailability limitations. This formulation may provide enhanced therapeutic outcomes and improved patient compliance in the treatment of GERD.

Keywords: Vonoprazan fumarate, Nanostructured lipid carriers, Gastroesophageal reflux disease, P-CAB.



PD-DB-044: A Study on Bioavailability Enhancement of Alendronate by using Natural Bioenhancers: for Effective Treatment of Osteoporosis

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Background: Osteoporosis is defined by reduced bone mass, density, and deterioration of bone microarchitecture. While bone formation initially outpaces resorption, this reverses by around the third decade of life, leading to net bone loss and increased fracture risk. Bisphosphonates (bps) are frontline therapies for postmenopausal osteoporosis and metabolic bone disorders, including glucocorticoid-induced bone loss. Alendronate, a low-lipophilicity, highly polar BP, is water-soluble but has poor oral absorption (0.59-0.64%) with wide inter- and intra-individual variability. It must be taken at least one hour before meals for optimal bioavailability. Bioenhancers are agents that enhance drug bioavailability and should be cost-effective, safe, fast-acting, reproducible, and compatible with active pharmaceutical ingredients (apis). By increasing absorption, bioenhancers can reduce required drug dosages, treatment cost, toxicity, and adverse effects.

Aims & Objectives: This study aimed to develop novel alendronate tablets incorporating natural bioenhancers—Aloe vera, niaziridin (from Moringa), Zingiber officinale (ginger), and glycyrrhizin (licorice)—to enhance alendronate's bioavailability and therapeutic efficacy. The formulated tablets were rigorously evaluated through pre-compression and post-compression characterization, including Drug content uniformity, weight variation, and assessments via *In-vitro* drug release and *In-vivo* studies.

Methods: Using direct compression, tablets were formulated with alendronate, natural bioenhancers, polyvinylpyrrolidone (as binder), and spray-dried lactose (as diluent). Evaluations included hardness testing, thickness measurement, friability, drug content, disintegration time, and dissolution profiling.

Results: Tablets hardness ranged from 4 to 5.5 kg/cm²; friability remained low at 0.6–0.7%. Thickness measured between 2.6–3.05 mm. Drug content averaged 90%, and disintegration times were within acceptable limits. The AZ₂ formulation demonstrated the highest *In-vitro* dissolution, achieving 54% alendronate release, a notable improvement over other formulations.

Conclusion: The AZ₂ formulation, enhanced with zingiber officinale(ginger) natural bioenhancers, substantially improved in vitro drug release. These promising results lay the groundwork for future in vivo pharmacokinetic evaluation to confirm enhanced absorption and therapeutic performance.

Keywords: Bioenhancers, Bioavailability, Zingiber officinale, Niaziridin, Aloe vera, Glycyrrhizin.



PD-DB-045: Formulation and Evaluation of Floating Tablets Using Modified Tamarind Gum for Sustained Release of Carvedilol

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Background: Oral drug delivery is the most widely used route due to its patient compliance. However, conventional immediate-release formulations present drawbacks such as frequent dosing for short half-life drugs and poor adherence, potentially leading to under- or over-medication, especially with narrow therapeutic index drugs. To address these issues, floating drug delivery systems offer prolonged gastric retention and sustained drug release.

Aims & Objectives: To develop and evaluate floating tablets of Carvedilol using chemically modified tamarind gum for sustained release.

Methods: Tablets were prepared by direct compression using carboxymethyl tamarind gum (CMTG), alone and with HPMC K4M as matrix-forming agents and sodium bicarbonate as gas forming agents. FTIR was used to assess drug-excipient compatibility. In vitro floating behavior and drug release kinetics were studied.

Results: Drug release varied significantly across formulations. F10 (7.82 mg CMTG + 23.43 mg HPMC K4M) showed the highest release ($96.31 \pm 0.39\%$) over 8 hours, followed by F8 ($73.12 \pm 0.77\%$) and F12 ($64.01 \pm 0.66\%$). Formulation F10 also demonstrated optimal floating behavior (lag time: 52 seconds; duration: >12 hours). Formulation F2, containing only CMTG, exhibited prolonged floating and $54.71 \pm 0.56\%$ drug release, following zero-order kinetics with anomalous (non-Fickian) diffusion. Increased CMTG concentration was inversely related to drug release. FTIR studies confirmed no significant drug-excipient interactions.

Conclusion: Modified tamarind gum (*Tamarindus indica*) from the Leguminosae family is effective for sustained-release floating tablets. Formulation F2 remained stable under accelerated conditions and shows potential for prolonged Carvedilol delivery.

Keywords: Carvedilol, floating tablets, tamarind gum, sustained release, FTIR, zero order kinetics.



PD-DB-046: Development of Dexamethasone-loaded Multilayer Nanofiber Based Ocular Inserts (MLNOI) for effective treatment of ocular inflammation

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Ocular inflammation is the immune response or irritation affecting parts of the eye, such as the conjunctiva, cornea, or uvea, often caused by infections, allergies, or autoimmune conditions. If left untreated, it can lead to serious complications such as tissue damage, vision impairment, or even permanent vision loss, making timely and effective treatment essential. The ocular inflammation presents a significant therapeutic challenge due to the complex anatomy and protective barriers of the eye, which hinder effective drug delivery and retention. Nanofibers offer better ocular surface retention and sustained drug release than conventional formulations and other nanocarriers, making them especially effective for treating ocular inflammation. To tackle with this, we developed a multilayer nanofiber-based ocular insert (MLNOI) for sustained and localized delivery of **Dexamethasone**, a potent corticosteroid with well-established anti-inflammatory efficacy. The inserts were fabricated via a sequential electrospinning process, resulting in a layered structure comprising **polyvinyl alcohol (PVA)**, **polycaprolactone (PCL)**, and **PVA**. This configuration was optimized to achieve enhanced mechanical stability, bioadhesion, and sustained drug release. Comprehensive physicochemical characterization confirmed uniform fiber morphology, desirable thickness, and drug encapsulation efficiency. ***In vitro* release** exhibited biphasic release pattern sustained over 24 h. MLNOI exhibited high permeability across goat cornea. The formulation passed **sterility, isotonicity, and HET-CAM** tests, confirming ocular safety. ***In vivo* pharmacokinetic studies** in rabbit model demonstrated significantly prolonged ocular residence time compared to standard eye drops. **Pharmacodynamic studies** showed rapid recovery from inflammation, and **stability tests** confirmed formulation robustness over four weeks. These findings support the potential of the developed MLNOI as a safe, and effective alternative for managing ocular inflammation.



PD-DB-047: Celecoxib Nanosuspension Based Gel for Topical Delivery

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Background: Celecoxib, a selective COX-2 inhibitor widely used for treating pain and inflammation in arthritis, causes gastrointestinal (GI) bleeding when administered orally due to its poor aqueous solubility and systemic exposure; therefore, it is formulated as a nanosuspension and delivered via the topical route to enhance solubility and minimize GI complications.

Aims & Objectives: The objective was to develop and evaluate a Celecoxib nanosuspension-based topical gel to overcome first-pass metabolism and gastrointestinal side effects, and to enhance dermal permeation.

Methods: Celecoxib nanosuspension was prepared using a media milling technique with zirconium oxide beads, Poloxamer 188 as a stabilizer, and Tween 80 as a surfactant. The nanosuspension was incorporated into a gel using polymers such as HPMC K4M and sodium alginate. The gel was evaluated for pH, spreadability, drug content, and in vitro permeation.

Results: Among the developed formulations, CN1 showed optimal characteristics with a particle size of 992.8 nm, PDI of 0.880, and zeta potential of -12.6 mV. The gel formulation (CGF1) showed a pH of 7.1 ± 0.3 , drug content of $94.77 \pm 0.24\%$, and spreadability of 5.6 ± 0.37 cm. In vitro studies indicated 63.86% drug release in 6 hours. The drug release followed first-order kinetics and non-Fickian diffusion mechanism.

Conclusion: The Celecoxib nanosuspension-loaded topical gel demonstrated controlled release and improved skin permeation, offering a promising non-oral alternative for long-term anti-inflammatory therapy.

Keywords: Celecoxib, nanosuspension, topical gel, media milling, drug permeation, COX-2 inhibitor.



PD-DB-048: A study on the use of modified chitosan for colonic delivery of secnidazole.

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Background: Secnidazole is a poorly soluble antiprotozoal drug that requires targeted release in the colon for effective therapeutic action. Colon-targeted delivery can improve drug efficacy and reduce systemic side effects. Chitosan, a natural polymer, was modified into succinate and phthalate derivatives to improve performance as a carrier.

Aims & Objectives: The aim of this study was to formulate a colon delivery system for secnidazole using modified chitosan polymers as binding agents, and to evaluate its potential in controlling drug release at the colon site.

Methods: Modified chitosan derivatives were used at concentrations of 3% to 25% for preparing secnidazole core tablets and the tablets were compression coated with HPMC K4M. The prepared tablets were evaluated for drug content, physical characteristics, swelling index and in vitro drug release. Drug release was studied in simulated gastric fluid (0.1 N HCl, pH 1.2) and simulated intestinal fluid (PBS, pH 6.8). FTIR analysis was performed to check drug-excipient interaction.

Results: The core tablets containing chitosan and modified chitosan showed 37.15 ± 1.67 to $97.43 \pm 0.07\%$ during 8h of dissolution testing. The tablets compression coated with HPMC exhibited release of 34.15 ± 5.3 to $82.80 \pm 3.7\%$ drug release. It was observed that on compression coating the release was reduced significantly during the first 4 hours where drug release was in range of 6.12 ± 1.2 to $7.87 \pm 1.7\%$. The degree of substitution for the modified chitosan was determined to be 17.52% and 19.41 %, respectively for succinate and phthalate derivatives. The drug release followed zero order kinetics and fickian mechanism.

Conclusion: The study demonstrated that modified chitosan derivatives effectively controlled secnidazole release and ensured colon targeting. These findings support the potential of chitosan succinate and chitosan phthalate in colon-specific drug delivery.

Keywords: Secnidazole, colon-targeted delivery, chitosan succinate, chitosan phthalate, compression-coated tablets, HPMC K4M.



PD-DB-049: Formulation and evaluation of quercetin loaded silver nanoparticles in hydrogel for effective treatment of acne

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Background:

Acne vulgaris is one of the most widespread dermatological conditions, affecting nearly 80% of adolescents globally at some point in their lives. Repeated use of antibiotics for treatment often leads to bacterial resistance, limiting the effectiveness of conventional therapies. Quercetin, a naturally occurring flavonoid, has been historically recognized for its medicinal properties, particularly its antibacterial activity. With increasing interest in herbal and nanotechnology-based treatments, the integration of quercetin into modern topical formulations offers promising potential.

Aims & Objectives:

The main objective of this study was to explore the green synthesis of quercetin-based silver nanoparticles and to formulate a herbal topical gel for the treatment of acne vulgaris. The study aimed to assess the physical characteristics and antibacterial efficacy of the developed gel, particularly against *Propionibacterium acnes*.

Methods:

Silver nanoparticles were synthesized using a green synthesis method, where 1 mM aqueous silver nitrate solution was reduced using quercetin. The formation of nanoparticles was confirmed through UV-visible spectroscopy. The nanoparticles were characterized for shape, size, and stability. These synthesized nanoparticles were then incorporated into a gel base, which was evaluated for pH, viscosity, spreadability, and antibacterial activity against *Propionibacterium acnes*.

Results:

The synthesized quercetin silver nanoparticles were spherical and stable, with an average particle size of 94.34 nm and a polydispersity index (PDI) of 0.307. The herbal gel formulation showed excellent physical characteristics, including smooth texture without any lumps or fibers, uniform color distribution, and good spreadability. The pH ranged between 6.71 ± 0.04 to 7.10 ± 0.02 , aligning well with the natural pH of human skin. Antibacterial testing revealed that the gel exhibited significant inhibitory effects against *Propionibacterium acnes*. Notably, the quercetin silver nanoparticle gel displayed greater antibacterial activity than both pure quercetin and plain silver nanoparticles.

Conclusion:

The study concludes that the green-synthesized quercetin silver nanoparticles incorporated into a topical gel base show promising antibacterial activity against acne-causing bacteria. This herbal nanoparticle-based gel formulation holds potential as an effective and skin-compatible alternative for the treatment of acne vulgaris.

Keywords:

Quercetin, Anti-acne, Silver nanoparticles, Herbal gel, Topical formulation, *Propionibacterium acnes*.



PD-DB-050: qbd-Driven Design of Calendula Essential Oil Nanosponge Topical Gel for Enhanced Antibacterial Efficacy

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Background: The increasing incidence of multidrug-resistant (MDR) infections caused by *Staphylococcus aureus* and *Escherichia coli* has heightened the need for novel antibacterial formulations. *Calendula essential oil* (CEO) possesses broad-spectrum antibacterial properties but suffers from low aqueous solubility, poor stability, and uncontrolled release, limiting its therapeutic efficacy. Nanosponge-based drug delivery systems offer promising potential for enhancing the performance of phytochemicals in topical applications.

Aims & Objectives: The objective of the present study was to design, optimize, and evaluate CEO-loaded nanosponges (CEO-NS) using a Quality-by-Design (qbd) approach and incorporate them into a topical gel formulation to improve antibacterial activity, stability, and controlled drug release.

Methods: CEO-NS were prepared using the emulsion solvent diffusion technique, using ethyl cellulose (EC) as the polymer and polyvinyl alcohol (PVA) as the stabilizer. A box-behnken design (BBD) was utilized for the optimization of formulation variables. NS were characterized by particle size, polydispersity index (PDI), zeta potential (ZP), encapsulation efficiency (EE), Fourier-Transform Infra-Red spectroscopy (FTIR), and scanning electron microscopy (SEM). The chosen optimized formulations (NS18, NS19, NS20) were loaded into gels (G1, G2, G3) and tested for viscosity, ph, spreadability, homogeneity, *in vitro* drug release, and antibacterial activity.

Results: Among the formulations tested, NS18 was considered an ideal formulation with a particle size of 268.7 nm, a PDI of 0.421, ZP of -20.98 mv, and The predicted desirability of formulation NS18 was 1, while the actual experimental desirability was 0.9157, indicating excellent agreement and near-optimal performance. Which was an indicator of good colloidal stability. The percentage EE was between 78±1.6 and 92±2.2. SEM showed spherical porous morphology, and FTIR showed the absence of significant drug-excipient interactions. The G1 showed optimum physicochemical characteristics (viscosity: 3454.12–3678.23 cps; spreadability: 40.37–66.77 g/cm/sec; ph: 5.2–5.7), The controlled drug release observed in G1 gel is a sustained release, where the drug is released at a steady rate over 8 hours. It follows the Hixson-Crowell model and has better antibacterial activity against *Staphylococcus aureus* (S. Aureus) and *Escherichia coli* (E. Coli) than pure CEO.



Conclusion: The topical gel (G1) controlled the release of the drug with improved antibacterial efficacy, making it a promising formulation for topical antibacterial therapy.

Keywords: *Calendula* essential oil, Nanosponge, Box-Behnken Design, Antibacterial activity.



PD-DB-051: Formulation and Evaluation of *Fumaria parviflora* Loaded Oil-in-Water Emulsion-Based Cream

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Background: *Fumaria parviflora* Lam. (Papaveraceae) is a medicinal herb traditionally used for treating skin infections such as folliculitis and erysipelas. The plant exhibits antibacterial, diuretic, and blood-purifying properties, making it a suitable candidate for topical formulation.

Aims & Objectives: To formulate an oil-in-water (o/w) emulsion-based cream loaded with *Fumaria parviflora* extract and evaluate its physicochemical, antibacterial, and antifungal properties for potential dermatological application.

Methods: The ethanolic extract of *Fumaria parviflora* was prepared using Soxhlet extraction. The o/w cream was formulated by emulsifying the oil and aqueous phases followed by evaluation of pH, viscosity, spreadability, thermal stability, irritancy, and phase separation. Antibacterial activity was assessed against *Staphylococcus aureus* and *Escherichia coli*, while antifungal efficacy was tested against *Candida albicans* and *Fusarium oxysporum*.

Results: The formulated cream exhibited pH 5.6 (skin-compatible), good spreadability, viscosity (1000–3000 cp), and thermal stability without phase separation. The formulation showed significant antibacterial activity with inhibition zones against *S. Aureus* and *E. Coli* but negligible antifungal effect.

Conclusion: *Fumaria parviflora* o/w emulsion-based cream demonstrated promising antibacterial properties and physicochemical stability, suggesting its potential use as a topical treatment for bacterial skin infections.

Keywords: *Fumaria parviflora*, oil-in-water emulsion, antibacterial cream, topical formulation, skin infections.



PD-DB-052: Formulation and Evaluation of Epigallocatechin Gallate Herbal Cream for Improved Management of Common Warts

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Common warts, caused by human papillomavirus (HPV), are benign proliferative skin lesions that can cause discomfort, recurrence, and aesthetic concerns. Conventional treatments like salicylic acid and cryotherapy often present limitations including prolonged therapy, irritation, or scarring. This research focuses on the formulation and evaluation of a topical herbal cream incorporating Epigallocatechin gallate (EGCG), a potent polyphenol derived from green tea, known for its antiviral, antioxidant, and anti-inflammatory properties. The study aimed to develop an oil-in-water (O/W) cream combining EGCG and salicylic acid to enhance therapeutic efficacy and patient compliance in wart management. Pre-formulation studies included FTIR, DSC, and molecular docking to confirm drug compatibility and target interactions. The cream was evaluated for physicochemical parameters such as pH, viscosity, spreadability, drug content, in vitro diffusion, and stability. MTT assay confirmed its biocompatibility. The optimized formulation exhibited superior diffusion characteristics, good stability, and promising anti-viral action, suggesting synergistic activity between EGCG and salicylic acid. The study concludes that the novel EGCG-based cream offers a safe, effective, and cosmetically acceptable alternative for managing common warts, potentially overcoming limitations of conventional therapies while utilizing a plant-based bioactive agent.

Key words: Epigallocatechin gallate (EGCG), Human papillomavirus (HPV), Herbal cream, Salicylic acid, Antiviral agent, Skin lesions, Natural polyphenol, FTIR, In vitro diffusion, MTT assay, Dermatological therapy, Green tea extract.



PD-DB-053: Natural phytochemical and biological activities of opuntia ficus-indica

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Remember that everyone's skin type and issues are different, so choose cactus-based products that are right for you. Listen to your skin and tweak your routine as necessary to attain the greatest results. If have specific skin disorders or concerns, by taking tailored advice on incorporating cactus extract into skin care routine.

Because of its multiple skin advantages, cactus, notably prickly pear cactus (opuntia ficus-indica), has become a popular ingredient, has popular ingredient in cosmetics utilising the power of cactus in skincare. Peel patch tests to check compaibility, and combine them with a well-rounded skincare programme that includes washing and sun protection. The prickly pear cactus (Opuntia ficus-indica) is known as "Nature's hydration Maestro" it provides and retain moisture. Cactus is famous for its hydrating properties, which include high water content, natural moisturizing factors, hyaluronic acid-like properties, skin barrier support, long lasting hydration soothing and calming, non-greasy structure, organic and natural options. Cactus extract contain flavonoids, which are antioxidants. They prevent skin damage from free radicals brought on by environmental toxins and uv rays and cactus based products to have anti-aging and skin brightening properties. Betalains vivid pigments found in cacti that are responsible for certain species they have anti-inflammatory and antioxidant qualities that may help reduce skin redness and irritation. Amino acids and Vitamins found in cactus extract include vitamin C, vitamin A, and vitamin E these promotes skin health. Calcium and magnesium are two minerals found in cactus extract helps to maintain skin health. Polyphenols containing cactus extract have antioxidants and anti-inflammatory effects.

Key words: Prickly pear cactus, Cactus extract, Skin barrier support, Long lasting moisture, Anti-aging, Anti-inflammatory, Anti-oxidants, Nutritional Elements as Vitamins, Calcium, Magnesium.



PD-DB-054: Engineering TRAIL-Conjugated slns for Oxaliplatin Delivery: A Step Toward DR4/DR5-Targeted Colorectal Cancer Therapy

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Background: Conventional chemotherapy is frequently limited by systemic toxicity and poor tumour selectivity, making colorectal cancer one of the leading causes of cancer mortality. Through DR4/DR5 receptor-mediated pathways, TRAIL (Tumour necrosis factor-related apoptosis-inducing ligand) has shown promise as a tool for selectively causing apoptosis in cancer cells.

Aims & Objectives: To develop a receptor-targeted hybrid nanocarrier system of oxaliplatin-loaded solid lipid nanoparticles (slns) conjugated with TRAIL to enhance selective cytotoxicity and bioavailability in colorectal cancer therapy.

Methods: Solid lipid nanoparticles were prepared by a modified microemulsion method using glyceryl monostearate, DDAB, and soya lecithin with Tween 80 as a stabilizer. Optimization was achieved via Box-Behnken Design based on particle size, PDI, and zeta potential. Pegylation were performed through EDC/NHS chemistry, TRAIL conjugation happened via Electrostatic Interaction and confirmed via FTIR, SDS-PAGE, UV-Vis spectroscopy, ELISA, and zeta analysis. In vitro cytotoxicity was evaluated on Caco-2 and HCT-15 cells, and in vivo efficacy and biodistribution studies were carried out in xenografted nude mice.

Results: The optimized TRAIL-conjugated slns displayed particle size <150 nm, narrow PDI, and stable surface charge. Conjugation was successfully confirmed through multiple physicochemical and biochemical techniques. In vitro studies showed significantly enhanced cytotoxicity and apoptosis induction compared to free oxaliplatin and non-conjugated formulations. The nanoparticle system triggered cell cycle arrest and elevated expression of pro-apoptotic markers such as BAX, BAD, and Caspase-3, validating its mechanistic potential in targeted cancer therapy.

Conclusion: The developed TRAIL-conjugated oxaliplatin-loaded slns demonstrated promising in vitro anti-cancer efficacy, enhanced cellular uptake, and selective apoptotic activity in colorectal cancer cell lines. These findings establish a strong preclinical foundation for further in vivo evaluation and potential translational development.

Keywords: TRAIL, Oxaliplatin, Solid Lipid Nanoparticles, Colorectal Cancer, Targeted Drug Delivery, Apoptosis, Receptor-Mediated Therapy



PD-DB-055: qbd- Driven development of Transfersomal gel system for targeted Transungual therapy in Onychomycosis

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Onychomycosis, a nail unit fungal infection, is challenging to treat because the nail's tough keratin structure prevents medications from passing through. It commonly returns. Common oral antifungals can harm the body and don't always work. This study introduces a gel system with transfersomes to overcome transungual drug delivery issues. A mucoadhesive gel with film-forming and moisturizing ingredients retains the medicine in the nail longer and hydrates the area, softening the nail barrier and allowing the drug to diffuse. We optimized the formulation process with Quality-by-Design (qbd). We examined important formulation variables that affect vesicle size and entrapment efficiency using a Box-Behnken design. The *in-vitro* antifungal activity showed better inhibitory zones than conventional gels. System stability testing demonstrated even greater stability. This multi-functional, patient-friendly platform could revolutionize topical nail therapy by enabling localized, long-lasting, and targeted administration without systemic exposure.



PD-DB-056: Nanoemulgel-Based Transdermal Delivery of JAK Inhibitor Tofacitinib for Localized Rheumatoid Arthritis Therapy.

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Background: Rheumatoid arthritis (RA) is a severe inflammatory disease characterized by persistent joint pain, inflammation, and increasing impairment of function. Due to non-specific distribution, systemic administration of therapeutic medicines such as tofacitinib frequently produces systemic adverse effects and inferior efficacy. Topical nanoformulations provide localized therapy with less systemic exposure and better medication targeting.

Aims & Objectives: The Aim and objective of this study was to improve therapeutic efficacy and patient compliance in the treatment of RA by designing and refining a transdermal nanoemulgel formulation of tofacitinib utilizing a Taguchi orthogonal array.

Methods: Tofacitinib was used to create a topical nanoemulgel, which was then refined using a L6 (3^4) Taguchi design. Three levels of variation were applied to four independent variables: oil concentration, S mix concentration, homogenization speed, and homogenization time. Nine formulations were evaluated for critical quality attributes such as in vitro drug release, entrapment efficiency (EE%), polydispersity index (PDI), and particle size. For in vivo anti-arthritic testing, the best run (Standard Order 2) was chosen.

Results: Particle size of 185.01 nm, PDI of 0.201, EE% of 70.12%, and drug release of 76.01% demonstrated excellent physicochemical properties in run 6. In vivo tests confirmed the formulation's anti-inflammatory properties by showing significantly lower arthritis scores at Day 14 in treated groups (low dose: 7.6 ± 0.9 ; high dose: 5.2 ± 0.6) as compared to arthritic control (12.8 ± 1.2).

Conclusion: S mix concentration and homogenization parameters were found to be important determinants of the nanoemulsion formulation, which was successfully optimized by the Taguchi technique. Tofacitinib nanoemulgel, which is the result, offers a promising non-invasive approach to targeted RA treatment with improved patient adherence and decreased systemic toxicity.

Keywords: Tofacitinib, Rheumatoid arthritis, Nanoemulgel, Topical drug delivery



PD-DB-057: Formulation and Evaluation of Amphotericin B-Loaded Cubosomes for Enhanced Antifungal Delivery

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Background: Ocular fungal infections, particularly fungal keratitis, present significant therapeutic challenges due to the poor aqueous solubility, limited corneal retention, and potential toxicity of conventional Amphotericin B (Amp B) formulations.

Aims & Objectives: This study aims to develop and evaluate Amp B-loaded cubosomes as a novel localized ocular drug delivery system to enhance bioavailability, retention, and antifungal efficacy.

Methods: Cubosomes were prepared by a top-down approach using glyceryl monooleate (GMO) and Poloxamer 407. Eight formulations (F1–F8) were developed and evaluated. F2, containing 2% GMO and 1% Poloxamer 407, was selected based on preliminary screening. The formulation was characterized for particle size, zeta potential, and entrapment efficiency. FTIR spectroscopy was used to confirm chemical integrity, while Scanning Electron Microscopy (SEM) was employed to investigate the surface morphology and structural characteristics of the optimized cubosomal formulation. Antifungal efficacy against *Candida albicans* was assessed through agar diffusion assay. Additionally, ex vivo transcorneal permeation studies were conducted using freshly excised bovine cornea mounted on a Franz diffusion cell. The results demonstrated enhanced permeation and prolonged retention of the cubosomal formulation compared to the plain drug solution, indicating its potential to improve localized ocular bioavailability.

Results: The optimized formulation F2 (2% GMO, 1% Poloxamer 407) exhibited a mean particle size of 163 ± 4.28 nm, a zeta potential of -23.1 ± 0.12 mv, and an entrapment efficiency of $82.21 \pm 0.12\%$, indicating a stable nanosystem with efficient drug encapsulation. FTIR spectroscopy confirmed the chemical integrity of Amphotericin B, with no observable interactions between the drug and excipients. SEM analysis revealed well-defined cuboidal structures with smooth surfaces and uniform particle distribution, confirming the successful formation of cubosomes. Antifungal activity evaluated via agar diffusion assay displayed a significantly larger zone of inhibition for F2 compared to a marketed Amphotericin B formulation, indicating enhanced efficacy against *Candida albicans*. Furthermore, ex vivo transcorneal permeation studies using sheep cornea mounted on a Franz diffusion cell showed improved drug permeation and prolonged ocular surface retention of the cubosomal formulation compared to the plain drug solution, suggesting enhanced bioavailability and localized therapeutic potential.

Conclusion: Amp B-loaded cubosomes represent a promising, stable, and biocompatible ocular drug delivery system with enhanced therapeutic potential for the treatment of fungal keratitis.

Keywords: Amphotericin B, Fungal keratitis, Antifungal activity



PD-DB-058: Black Seed Oil and Rose Hip Oil Based Nanoemulgel for the Effective Treatment of Acne Including Scars.

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Background: Acne is a topical inflammation it may be caused by hormonal, environmental or by certain bacteria called *P. Acne* in the presence of excess secretion of sebum. Though the condition is not life threatening, it effects the patient both psychologically as well as psychosocially. The conventional treatment methods ends in leaving behind the scar and hyper-pigmentation. The present novel lipid-based technology containing retinoid with oils like black seed oil and rose hip oil for treating acne including scars.

Aims & Objectives: To develop and characterize nanoemulsion gel using black seed and rose hip oil with retinoid for the effective management of acne including scars.

Methods: Preformulation studies were performed for the estimation of calibration curve, stability studies and FTIR compatibility studies and then nanoemulsion preparation was done by using spontaneous emulsification method and then characterization of prepared nanoemulsion was done by using spontaneous emulsification method and then characterization of prepared Nanoemulsion for obtaining thermodynamic stability, particle size, etc. And then selection of gelling agent and incorporation of nanoemulsion, characterization for Nanoemulsion gel viscosity, extrudability and further carried out for *in-vivo* skin irritation study and treatment of pustules with prepared and marketed product.

Results: All the studies have shown appropriate results which is the action that can be shown on reducing acne scars, and further There was no skin irritation, redness, or erythema observed during this study. Since the prepared formulation is a nanoemulsion and it had a capacity to penetrate easily into the stratum corneum as compared to the marketed formulation, thus producing a better efficacy.

Conclusion: Drug and other excipients are compatible with each other. All the test parameters were passed by the formulation. The nanotechnology is implemented in these works, the formulation can cross stratum corneum easily and actually impact the area affected as it is a nanoemulsion. *In-vitro* studies of different types substantiating the efficacy of acne product.

Keywords: Acne scars, Nanoemulsion, gel, Characterization.



PD-DB-059: Development and characterization of papain loaded oral dispersible strips/films for treatment and management of oral mucositis
Shakthi Priyan S

Cancer therapies such as chemotherapy and radiotherapy are widely employed for the treatment of various malignancies. However, these aggressive treatment modalities often induce severe side effects, among which oral mucositis is a common and debilitating condition. Oral mucositis results in inflammation and ulceration of the mucosal lining, significantly impacting the patient's quality of life and leading to complications such as pain, difficulty in eating, and risk of infection. Conventional oral formulations like tablets and capsules are often prescribed to manage these symptoms, but they present several limitations. Patients experiencing oral mucositis frequently suffer from difficulty in swallowing, reduced drug efficacy due to limited local targeting, and only temporary symptom relief. Moreover, these formulations may induce additional adverse effects, further complicating the management of mucositis. To overcome these challenges, innovative drug delivery systems such as oral thin films (otfs) are emerging as a promising alternative. These films offer several advantages including ease of administration, rapid onset of therapeutic action, enhanced bioavailability, and minimized systemic side effects. Due to their mucoadhesive properties and ability to dissolve quickly in the oral cavity, otfs ensure direct contact with the affected mucosa, thereby providing localized and effective treatment. This novel approach not only improves patient compliance but also enhances therapeutic outcomes by targeting the site of action more precisely. The integration of otfs in the management of oral mucositis represents a significant advancement in supportive cancer care, offering a patient-friendly and efficient alternative to traditional oral dosage forms.

Key words: Oral mucositis, Chemotherapy, Radiotherapy, Cancer therapy side effects, Oral drug delivery, Oral thin films (otfs).



PD-DB-060: Formulation and Evaluation of Clopidogrel Bisulphate Floating Sustained Release Tablet

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Background: Clopidogrel Bisulphate is an antiplatelet agent used in the prevention of thrombotic events associated with peripheral vascular disease, coronary artery disease, and cerebrovascular disease. However, its therapeutic efficacy is limited due to its short half-life and low bioavailability (50%). To overcome these limitations, a floating drug delivery system was developed to enhance gastric retention and sustain drug release

Aims & Objectives: This study aimed to formulate and evaluate floating tablets of Clopidogrel Bisulphate using natural polymers (Chitosan and Pectin), a synthetic polymer (HPMC), and sodium bicarbonate as a gas-generating agent.

Methods: FT-IR analysis was conducted to assess drug-excipient compatibility. Tablets were prepared by direct compression and evaluated for physicochemical parameters, drug content, swelling index, in-vitro drug release, and release kinetics. In-vitro drug release studies were performed in 0.1N HCl to simulate gastric conditions.

Results: All formulations showed acceptable floating lag time and total floating duration. Among the formulations, F3 exhibited sustained drug release of $54.37 \pm 0.38\%$, likely due to the presence of higher concentration of Chitosan. Drug release from formulation F3 followed first-order kinetics and a non-Fickian diffusion mechanism.

Conclusion: The study concludes that the floating drug delivery system of Clopidogrel Bisulphate using natural and synthetic polymers can provide sustained drug release and potentially improve bioavailability.

Keywords: Clopidogrel Bisulphate, Chitosan, Pectin, Floating Drug Delivery System, HPMC, Sustained Release.



PD-DB-061: Chemoinformatics-Driven Machine Learning Models and Neural Network for Predicting Blood-Brain Barrier Penetration

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Introduction: Predicting whether a drug can cross the blood-brain barrier (BBB) is critical in developing central nervous system (CNS) therapeutics. Conventional methods are resource-intensive; hence, Artificial Intelligence (AI) presents an efficient alternative using chemoinformatic data.

Aim & Objective: To develop and evaluate AI models that predict BBB permeability from molecular structure representations.

Methods: We used the M³-20M dataset, and selected molecules labeled for BBB permeability. Data preprocessing included, handling missing values, and balancing class labels using Synthetic Minority Over-sampling Technique (SMOTE). Molecular structures were converted from Simplified Molecular Input Line Entry System (SMILES) to rdkit Mol objects and encoded as 2048-bit Morgan fingerprints (radius=2). Dimensionality reduction was performed using Principle Component Analysis (PCA), retaining 95% variance. Classifiers including Decision Tree, Random Forest, Support Vector Classifier (SVC), Logistic Regression, Neural Network, and a Stacking Classifier were implemented. Hyperparameter tuning was done using Gridsearchcv, and models were validated with 5-fold cross-validation.

Results: The stacking classifier demonstrated the best overall performance, achieving 95.1% accuracy, 0.94 precision, 0.95 recall, 0.95 F1-score, and 0.945 AUC. The model showed consistent generalization with a cross-validation mean accuracy of 94.8% $\pm$ 0.7%. SVC achieved 93.1% accuracy with an AUC of 0.931, and a mean cross-validation score of 93.9% $\pm$ 0.58%. Random Forest reached 92.8% accuracy, AUC 0.924. The neural network achieved 92% test accuracy, with validation accuracy stabilizing above 90% by epoch 12 and a minimum validation loss of 0.26. Logistic Regression also performed well with 91.1% accuracy and AUC 0.915.

Conclusion: AI models using chemoinformatic fingerprints provide accurate, scalable solutions for BBB permeability prediction, significantly aiding CNS-targeted drug discovery.

Keywords: Blood-brain barrier, drug discovery, chemoinformatics, machine learning, molecular fingerprints



PD-DB-062: Cardio-Films: Rapid Mucoadhesive Platforms for On-the-Go Drug Administration

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Background: Cardiovascular diseases (cvds) are the primary cause of mortality worldwide, requiring quick-acting and effective drug delivery. Buccal films hold a promising approach by avoiding hepatic first-pass metabolism, with quick onset, increased bioavailability, and better patient compliance. Recent research ventures into their potential use for delivering cardiovascular agents such as carvedilol, enalapril, ivabradine, and nitroglycerin.

Aim: To formulate and assess mucoadhesive buccal films for accelerated delivery of cardiovascular drugs, enhancing the pharmacokinetic performance and therapeutic outcome.

Method: Cardiovascular drugs were loaded into buccal films through solvent casting employing polymers such as HPMC, PVA, and Carbopol. The physicochemical and mechanical properties of films, drug content, in vitro release, mucoadhesive strength, and ex vivo permeation were assessed. In vivo pharmacokinetic tests were conducted on selected formulations.

Results: Movies indicated uniform distribution of drugs, quick disintegration, and maximum adhesion. They showed quick release and better mucosal absorption in in vitro and ex vivo studies. Carvedilol and enalapril films revealed increased bioavailability, while ivabradine films released sustained heart rate control.

Conclusion: Mucoadhesive buccal films are an effective, patient-friendly approach to cardiovascular drug delivery. They provide quick action and better compliance, with excellent potential for emergency applications and chronic care applications.

Keywords: Mucoadhesive buccal films, cardiovascular agents, bioavailability



PD-DB-063: Design, Formulation And Assessment Of Herbal Moisturizing Cream

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Aim: The aim of the study focuses on the Design, formulation and assessment of herbal moisturizing cream incorporating herbal ingredients by employing a systematic factorial design approach.

Methodology: The cream was formulated with extract of vetiver, cactus gel, and alpha hydroxy acids (AHA). Five different formulations (F1, F2, F3, F4, and an optimized formulation FM) were prepared by varying the amounts of herbal ingredient. Factorial design was employed to systematically evaluate the impact of varying concentrations of vetiver and AHA on key properties like pH and viscosity. This method allowed for a detailed analysis of ingredients and their effects on the cream's performance.

Results: The optimized formulation showed pH of 6.2 & viscosity of 78,154 cp, both indicative of stability and suitability for skin application. The microbial analysis of the cream was conducted to ensure safety and compliance. Total viable bacterial counts and total yeast and mould counts were found to be below 10 cfu/g indicating a low microbial load and suitability for cosmetic use. Importantly, tests for pathogenic bacteria including *E.coli*, *P.aeruginosa* and *S.aureus* returned negative results, confirming the absence of microorganisms. The heavy metal analysis revealed that lead content ranged from 0.032 to 0.053 ppm, while arsenic levels varied between 0.0020 and 0.0042 ppm. Both metals were found to be within acceptable limits, indicating that the formulations do not pose a risk of heavy metal toxicity.

Conclusion: The development of the herbal moisturizing cream utilizing herbal ingredients have demonstrated promising results in enhancing skin hydration and rejuvenation. This research highlights the efficacy of combining traditional herbal components with methodical formulation strategies also addresses common skin concerns, reaffirming the viability of herbal formulations in modern skincare.

Keywords: AHA, Cactus gel, Vetiver extract, Factorial Design



PD-DB-064: Formulation and evaluation of insitu forming gel for treatment of oral mucositis using model local anaesthetic drug

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Oral mucositis is a severe and painful side effect commonly observed in patients undergoing chemotherapy and radiotherapy, particularly for head and neck cancers. It compromises the mucosal barrier, leading to inflammation, ulceration, and increased infection risk. This study presents a thermosensitive, mucoadhesive in-situ gel (L-ISG) system for localized, sustained delivery of Lidocaine, a model local anesthetic, to effectively manage oral mucositis-associated pain. Lidocaine-loaded in-situ gels were formulated using the cold method and optimized via Central Composite Design by varying concentrations of Poloxamer 407 and Carbopol 934P. The optimized formulation demonstrated a rapid gelation time of 11.32 seconds and a gelling temperature of 37 °C, ideal for buccal application. The gel was clear, pH-balanced (6.8), and exhibited strong mucoadhesive properties and suitable viscosity (240.2 cps). In vitro drug release studies showed a sustained release of 83.3% over 8 hours, significantly outperforming plain drug solution, which released 90% in just 4 hours. Drug release followed zero-order kinetics ($R^2 = 0.9965$), indicating a controlled and concentration-independent release pattern. FTIR and DSC analyses confirmed no drug-excipient interactions and successful entrapment within the gel matrix. The developed mucoadhesive L-ISG offers site-specific delivery, enhanced mucosal residence time, and prolonged anesthetic effect, making it a promising, non-invasive approach for effective management of oral mucositis in cancer patients.

Keywords: Mucoadhesive in-situ gel, Lidocaine, Oral mucositis, Buccal drug delivery.



PD-DB-065: Green synthesis, characterization and gel formulation of silver nanoparticles using wild yam leaf extract

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Background: *Dioscorea villosa* (DV), known for its antibacterial properties. Bacterial infection treatment has been a major research priority in the pharmaceutical and personal care industries.

Aims & Objectives: The aim of the present work was to evaluate the phytochemical composition of *Dioscorea villosa* (DV), green synthesis and evaluation of silver nanoparticle and to develop herbal topical gel formulation to treat Bacterial infection.

Methods: Aqueous extract solution was prepared by the decoction method. Silver nanoparticles (agnps) were synthesized using 1mm silver nitrate with the extract as a reducing and capping agent. Agnp formation was confirmed by UV-Vis spectroscopy, with FT-IR, XRD, SEM, Particle size, and zeta potential confirming crystallinity and stability. The synthesized agnps were incorporated into a silver nitrate solution and evaluated for physical properties, including ph, viscosity, spreadability, and antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*.

Results: Phytochemical analysis of *Dioscorea villosa* extract showed alkaloids, flavonoids, tannins, and saponins. Silver nanoparticle was confirmed by UV spectroscopy. XRD patterns and zeta potential, respectively, confirmed the crystalline nature and stability of agnps. SEM revealed particle morphology. The gel showed smooth texture, uniform colour, easy washability, and good antibacterial efficacy. Suggesting its potential as an effective topical treatment for bacterial infections. It outperformed the marketed Silverex™ ionic gel, indicating its potential as a natural antibacterial treatment.

Conclusion: This study shows that *Dioscorea villosa*-mediated agnp gel (0.017% w/w) demonstrated a larger zone of inhibition against *E. Coli* and *S. Aureus* compared to the marketed 0.2% w/w silver nitrate gel, silverextm. Despite using 85% less silver, the formulated gel showed better antibacterial activity as compared to the marketed product due to its nanoparticle form, suggesting it as a more effective topical agent for treating bacterial infections.

Keywords: Green synthesis, silver nanoparticles, *Dioscorea villosa*.



PD-DB-066: Formulation and Evaluation of Oral Liposomal Glutathione: A Novel Antioxidant Delivery Approach

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Background and Objective: Glutathione (GSH), a powerful endogenous antioxidant, plays a critical role in maintaining redox homeostasis, immune function, and detoxification. However, its oral delivery is challenged by enzymatic degradation and poor bioavailability. This study was designed to develop and evaluate a liposomal formulation of glutathione intended for oral use, aiming to enhance its stability, bioavailability, and therapeutic potential.

Methodology: Glutathione-loaded liposomes were prepared using the thin-film hydration method and optimized using a 3^2 factorial design, with soya lecithin concentration and sonication time as key variables. The optimized formulation was characterized for particle size, zeta potential, entrapment efficiency, and morphology (TEM). Further, the liposomes were lyophilized and formulated into a dry syrup. In-vitro release studies and antioxidant activity (via DPPH assay) were conducted to assess performance.

Results: The optimized liposomes had a particle size of 139.08 nm, a zeta potential of -17.08 mV, and 72.18% entrapment efficiency. FTIR and DSC confirmed compatibility and thermal stability. TEM imaging revealed uniform spherical vesicles. The in-vitro release profile showed 75% drug release under intestinal pH conditions. The lyophilized dry syrup formulation had 89.43% drug content and maintained antioxidant activity, as confirmed by DPPH assay.

Conclusion: The liposomal formulation significantly improved the oral delivery and antioxidant efficacy of glutathione. The resulting dry syrup offers a patient-friendly, stable, and effective system for managing oxidative stress-related conditions.

Keywords: Glutathione, Liposomes, Oral Drug Delivery, Antioxidant, Dry Syrup, Thin-Film Hydration, Entrapment Efficiency.



PD-DB-067: Application of Sonocrystallization Technique for Solubility Enhancement of Etoricoxib

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Background: Etoricoxib is a non-steroidal anti-inflammatory drug belonging to BCS class II with poor water solubility (0.0767 ± 0.0018 mg/ml) resulting in limited oral bioavailability. It is used in the treatment of arthritis, gout, dental pain, and back pain. Improving solubility and dissolution behavior is essential for enhancing its therapeutic performance.

Aims & Objectives: The present study was aimed to enhance the solubility and dissolution rate of Etoricoxib using anti solvent sonocrystallization technique using cyclodextrin as complexing agent.

Methods: Etoricoxib crystals were prepared by the anti-solvent sonocrystallization method using ethanol as the solvent and water as the anti-solvent, where the drug solution was added dropwise into water. The recrystallization was performed under treatment of ultrasound (50% power, 2 duty cycle) for 5 minutes. In a modification of the method, beta cyclodextrin was added in the anti-solvent of the system, i.e., water to which drug solution was added dropwise under sonication. The crystals were filtered, dried at room temperature for 24 hours. The obtained crystals were evaluated for solubility, dissolution rate, morphology and drug–excipient interactions using FTIR.

Results: Among various formulations, the crystals prepared via anti-solvent sonocrystallization with beta cyclodextrin showed higher solubility and dissolution. The solubility of Etoricoxib in water, 0.1 N HCl and PBS (ph 6.8) was 80.16 ± 0.1326 , 168.83 ± 0.041 and 50.15 ± 0.021 mcg/ml, respectively. The solubility increased significantly to 103.25 ± 0.65 µg/ml (anti-solvent crystallization), 154.65 ± 0.83 µg/ml (anti-solvent sonocrystallization), and 330.54 ± 0.19 µg/ml with the beta-cyclodextrin complex. The dissolution study of pure drug exhibited 6% drug solution while the modified crystals exhibited a dissolution of 8.83 ± 0.0227 to $15.53 \pm 0.03\%$ in 60 mins. Microscopic analysis confirmed morphological changes in the crystals, while FTIR indicated potential interactions between Etoricoxib and beta-cyclodextrin.

Conclusion: The anti-solvent sonocrystallization method, especially when combined with beta cyclodextrin, is an effective approach to improve the solubility and dissolution rate of Etoricoxib, potentially leading to enhanced bioavailability.

Keywords: Etoricoxib, Anti-solvent sonocrystallization, Cyclodextrin, Solubility enhancement, Dissolution rate



PD-DB-068: Development And Evaluation Of Glycine Max Mucoadhesive Bioflexi Film Containing Valsartan Translabial Drug Delivery System

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Valsartan, a tetrazole derivative and angiotensin II receptor blocker, is widely used alone or in combination with other agents to treat hypertension and reduce cardiovascular mortality after myocardial infarction. Classified as a BCS Class II drug, its oral bioavailability is limited due to extensive first-pass metabolism and solubility issues. This study aimed to develop fast-dissolving thin films of Valsartan using different polymers and bio-adhesive excipients to facilitate immediate drug release via the translabial route, ensuring efficient and direct absorption into the systemic circulation. Pre-formulation studies confirmed the physical characteristics and compatibility of the drug excipients. Valsartan bio-flexi film was formulated with Glycine max and hydroxyl propyl methyl cellulose as polymers by solvent casting method and drug release was evaluated by egg shell membrane method. The drug release pattern exhibited a good fit to the Korsmeyer-Peppas model, with an r^2 value of 0.9955, indicating a reliable and predictable release profile. The release mechanism was identified as super case II transport, highlighting a polymer relaxation-driven and diffusion-controlled process. Among the tested formulations, GL1, comprising synthetic polymers, demonstrated the highest drug release of 81.12% at the end of 8 hours, making it the most effective and optimized formulation. These findings suggest that Valsartan-loaded thin films for translabial drug delivery hold significant promise as a novel and effective approach for the treatment of hypertension.

Keywords: Valsartan, Glycine max, HPMC E50, Bio-flexi film, Translabial route.



PD-DB-069: Improving Bioavailability of Rilpivirine Hydrochloride Using β -Cyclodextrin-Based Solid Dispersions

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Background: Rilpivirine hydrochloride, a BCS Class II antiretroviral drug, presents challenges in formulation due to its poor aqueous solubility, affecting its bioavailability. Enhancing its solubility is crucial for improving therapeutic efficacy and patient outcomes in HIV treatment.

Aims & Objectives: The study aimed to enhance the solubility and dissolution profile of Rilpivirine hydrochloride by formulating solid dispersions using hydrophilic carriers— β -cyclodextrin and Poloxamer 188—and to characterize the resulting formulations.

Methods: Solid dispersions were prepared via the kneading method in various drug-to-carrier ratios (1:2 to 1:8). The formulations were characterized using FTIR, DSC, PXRD, and SEM. In vitro solubility, dissolution, and release kinetics studies were conducted in phosphate buffer (ph 6.8) to evaluate performance.

Results: Among all formulations, the Rilpivirine: β -cyclodextrin (1:6) complex exhibited significantly improved saturation solubility (0.100 mg/ml) and dissolution (up to 104.67% in 150 minutes). Characterization confirmed inclusion complex formation with reduced crystallinity, enhanced wettability, and improved drug release.

Conclusion: Solid dispersion with β -cyclodextrin effectively enhanced the solubility and dissolution rate of Rilpivirine hydrochloride. This approach offers a promising strategy for improving the bioavailability of poorly soluble antiretroviral drugs.

Keywords: Rilpivirine Hydrochloride, Solubility Enhancement, Solid Dispersion, β -Cyclodextrin, Poloxamer 188, Inclusion Complex, Dissolution, BCS Class II.



PD-DB-070: Formulation and Evaluation of Peel-off mask using Cactus ficus-indica

Sajeeda banu M E

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PD-DB-071: A phase 1 trial for the evaluation of the safety and pharmacokinetics of islatravir subdermal implant for HIV-1 pre-exposure prophylaxis

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Background: Although there's a decline in HIV-1 mortality and transmission rates, an estimated 1.7 million new type 1 human immunodeficiency virus (HIV-1) infections occur annually, thus remaining a major global public health challenge. While approved daily oral pre-exposure prophylaxis (prep) regimens such as emtricitabine with tenofovir were effective, they showed variable tissue drug levels, and their success depends on strict patient adherence. To overcome these limitations, Islatravir, a long-acting nucleoside reverse transcriptase translocation inhibitor, is being developed for the prevention and treatment of HIV-1.

Aims & Objectives: This study aimed to conduct a randomized, double-blinded, placebo controlled, phase 1 trials in HIV-1 negative adults over 12 weeks to evaluate the safety, tolerability, and pharmacokinetic parameters of two prototypes of Islatravir subdermal implants (54 and 62 mg) to confirm whether the implant can maintain the intracellular concentrations above the required threshold.

Methods: Sixteen healthy adults (aged 18-55) were randomized to receive either islatravir or placebo implants placed in the upper non-dominant arm. Blood samples were collected at prespecified intervals to measure plasma islatravir and intracellular islatravir triphosphate concentrations. Pharmacokinetic parameters were analyzed using non-compartmental models. Safety was measured through clinical evaluations, lab tests, and aes (Adverse Events) monitoring.

Results: The reported aes were mild to moderate implant site reactions, such as erythema and tenderness, which almost resolved by the end of the study. Furthermore, the mean concentrations of islatravir triphosphate in Peripheral Blood Mononuclear Cells (pbmcs) were above the predefined efficacy threshold (>0.05 pmol/ 10^6 cells) throughout the 12-week trial, suggesting potential for therapeutic reverse transcriptase inhibition. The concentrations at day 85 for 54 mg and 62 mg were 0.135 and 0.272 pmol/ 10^6 cells, respectively.

Conclusion: These islatravir implants were long-acting, safe, tolerable, and had an optimum pharmacokinetic profile. Therefore, these required further investigation as a potential HIV prevention strategy.

Keywords: Human Immunodeficiency Virus, Pre-exposure Prophylaxis, Islatravir, Subdermal Implant, Pharmacokinetics.



PD-DB-072: Pharmacogenomic Variability in Beta-Blocker Response in Hypertension: A Meta-Analysis of ADRB1, CYP2D6, and GRK4 Variants

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Background: Individual responses to hypertension treatment vary widely, primarily due to genetic differences that affect drug metabolism and therapeutic outcomes. Pharmacogenomic variations in genes such as ADRB1, CYP2D6, and GRK4 play a key role in modulating the efficacy, safety, and dosing of antihypertensive agents. A thorough understanding of these gene-drug interactions is essential to tailor personalized treatment strategies and improve clinical outcomes in hypertension management.

Aims & Objectives: This meta-analysis examines genetic polymorphisms influencing beta-blocker response, aiming to quantify genotype-specific effects and assess ethnic differences in antihypertensive treatment outcomes.

Methods: A systematic literature search was conducted in pubmed, Web of Science, and Cochrane Library, supplemented with data from pharngkb, and dbsnp. Eligible studies included rcts, cohort, and case-control designs reporting antihypertensive response stratified by genotype. Data extraction captured study design, population, gene/SNP details, drug, clinical outcomes and effect sizes. Quality assessment followed JBI tool. Meta-analyses were performed using random effects models based on heterogeneity (I^2).

Results: A meta-analysis of eight pharmacogenomic comparisons revealed a significant association between genetic variants and beta-blocker response. The pooled odds ratio was 1.22 (95% CI: 1.10–1.36), indicating increased odds of efficacy or altered dosing based on genotype. Substantial heterogeneity was observed ($I^2 = 75.15\%$). Notably, ADRB1 rs1801253 showed consistent positive effects, while CYP2D6 variants influenced metoprolol dosing. These findings support the clinical relevance of pharmacogenomic-guided beta-blocker therapy.

Conclusion: Pharmacogenomic variants significantly influence antihypertensive response. Incorporating genetic data into therapy decisions can enhance treatment effectiveness and reduce side effects, reinforcing the role of personalized medicine in optimizing hypertension management.

Keywords: Pharmacogenomics, Antihypertensives, ADRB1, CYP2D6, Personalized medicine, Beta-blockers, Genetic polymorphism.



PD-DB-073: Precision in the Buccal Pocket: A Case Study on the Use of 3D-Printed Levetiracetam Films in Paediatric Epilepsy

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Background: Children with epilepsy continue to have difficulty adhering to medication, particularly with swallowing issues and taste intolerance. Traditional oral suspensions are among the most frequent causes of dosing omissions and affect seizure control and quality of life. Customized 3D-printed drug delivery devices have been shown to be an effective solution to overcome these problems.

Aims and Objectives: To determine the clinical effectiveness, drug kinetics, and patient acceptability of a newly developed 3D-printed buccal film drug delivery system of levetiracetam in a pediatric patient with refractory epilepsy with poor compliance to drugs.

Methods: An 18-kg 6-year-old boy with generalized tonic-clonic epilepsy, who had been taking oral levetiracetam suspension 500 mg/day, was converted to a 3D-printed buccal film releasing 250 mg levetiracetam twice daily. The hydroxypropyl methylcellulose and glycerol matrix film was flavoured and engineered to disperse rapidly in the mucosa. Pharmacokinetically sampled levetiracetam, seizure frequency, and caregiver rated palatability/compliance scores were compared over four weeks.

Results: Buccal film showed similar pharmacokinetic properties as oral suspension (C_{max}: 13.5 µg/ml; T_{max}: 1.2 hrs; AUC₀₋₄: 108 µg·h/ml; ~98% bioavailability). Seizure frequency decreased from 3–4/month to zero. Palatability, use, and caregiver satisfaction improved from 2–3 to 5 on a 5-point Likert scale. No side effects.

Conclusion: Buccal film 3D printing enhanced drug compliance and seizure control in a pediatric patient to a remarkable degree, proving the capability of personalized drugs to alleviate formulation issues. The procedure is a valid clinical use of 3D printing technology in pediatric drug therapy, which must be studied in larger populations.

Keywords: Paediatric Epilepsy, 3D Printing, Buccal Film, Levetiracetam, Personalized Pharmaceutics, Drug Adherence, Clinical Pharmaceutics



PD-DB-074: Management of atherosclerosis by formulating and optimizing nanotheranostic particle using Design of Experiment approach

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Background: Atherosclerosis is one of the leading causes of death due to non-communicable diseases. The progression of atherosclerosis might lead to several other complications, such as myocardial infarctions, stroke and congestive heart failure. Lipid-based nanotheranostic particles with suitable drug and imaging agents can be implemented to study the extent of the atherosclerotic plaques, and based on the imaging, the treatment can be altered. Design of Experiments (doe) is implemented to study the effect of different concentrations of different lipids and the homogenization speed on the particle size of the lipid-based nanotheranostic particle with the help of a central composite design (CCD).

Aims & Objectives: To develop a nanotheranostic particle for the imaging and therapy of atherosclerosis using the doe method. In-silico studies for choosing optimal ligand, Formulation of drug and imaging moiety loaded hybrid nanotheranostic particle. Optimization of the hybrid nanotheranostic particle using doe method. Characterization of the hybrid nanotheranostic particle. In-vitro and in-vivo studies of the hybrid nanotheranostic particle.

Methods: The methodology is initiated by identifying a suitable target. Once the target was identified, in-silico docking studies were carried out with a few drug molecules and the promising ones were chosen. Blank lipid-based nanoparticles were optimized using the CCD model with different lipid ratios as the factors. After optimization, they are loaded with the drug of choice and tagged with an imaging agent and the nanotheranostic particle is subjected to characterization and evaluation tests.

Results: The target has been identified as the LOX-1 receptor, and for that, Ligand binding studies were conducted with different molecules. The promising molecules have been shortlisted, and the same is being studied for in-vitro results.

Conclusion: The docking studies show promising results, and the same is expected in the in-vitro studies. If the results are favorable, the promising molecules can be used to develop a nanotheranostic particle for managing atherosclerosis.

Keywords: Nanotheranostics, atherosclerosis, Design of Experiments, LOX-1, Polymeric Nanoparticles



PD-DB-075: Folate-Conjugated Jacalin as a Potocytosis-Driven Therapeutic Strategy for Targeting Breast Cancer

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Background: Breast cancer is one of the most prominent cancer worldwide, with its main target population being the female population. It is the second largest cause of death worldwide among women. Various drugs and treatments have been developed to treat the different types of breast cancer based on the expression of specific surface receptors. A crucial and relatively well-researched element of the cell, called the caveolae, possesses a suitable delivery medium for small to medium-sized molecules across the cell membrane. Caveolae are small flask invagination in the cellular membrane and act as mediators of signal transduction, working closely with the Golgi apparatus. Act as lipid rafts, molecular transport, and endocytosis of molecules through a folate receptor-mediated pathway that is independent of the clathrin-coated pit mechanism. This process is called potocytosis.

Aims & Objectives: Potocytosis provides a potential drug delivery mechanism for transporting Jacalin, a well-researched and classified protein, to be delivered into the tumor and induce apoptosis, autophagy, and anti-inflammation.

Methods: To successfully deliver jacalin into the cell membrane potocytosis mechanism would be used. However, to initiate this endocytosis of jacalin, it must be linked with a folate molecule while keeping the lectin carbohydrate binding site free. This would be done using site-specific conjugation of jacalin with folate using an amino acid such as cystine away from its lectin pocket and linking it to the folate molecule. The new jacalin folate complex would interact with the GPI folate receptor clusters commonly found near the caveolae, leading to the formation of an intracellular vesicle from which the jacalin protein diffuses and interacts with the various macromolecules to initiate apoptosis.

Results: Jacalin, once inside the cytoplasm, would lead to binding to various glycol proteins, hindering cellular functioning, leading to apoptosis and anti-cancer properties, which the jacalin in the tumor microenvironment would induce anti-inflammatory properties.

Conclusion: Folate Jacalin conjugates may offer a novel receptor-targeted strategy for breast cancer therapy by selective delivery using potocytosis.

Keywords: Breast cancer, Folate receptor, Potocytosis, Jacalin, GPI (Glycosylphosphatidylinositol), Caveolae, Lectins, Targeted delivery.



PD-DB-076: Lactoferrin-Functionalized Liposomes for Co-Delivery of Baicalein and Galantamine: A Multi-Target-Directed Ligands Approach for Alzheimer's Disease Therapy

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Background: Alzheimer's Disease is a neurodegenerative disorder affecting the elderly population worldwide. The pathological hallmarks include the formation and accumulation of Amyloid-beta proteins extracellularly and Neurofibrillary tangles (nfts) intracellularly. Conventional therapies offer symptomatic relief rather than addressing the underlying pathological cause of the disease progression. Prevention of neurodegeneration will be a promising strategy for the management of AD. Many targets implicated in AD are identified as a strategy for preventing neurodegeneration in AD, including Beta-secretase (BACE1), Protein kinases, mtor, Caspase, Cellular Prior Protein, and Apolipoprotein, which are being explored widely. Single-target drugs often fail due to AD's multifactorial nature, necessitating a multi-targeted therapeutic approach. Recent clinical evidence supports the advantages of multi-targeting strategies in drug development for AD. This approach offers better therapeutic activity and reduces the peripheral side effects by simultaneously targeting amyloid-beta production and accumulation, tau hyperphosphorylation, and cholinergic deficits.

Aims & Objectives: The study aims to formulate and optimize lactoferrin-functionalized liposomes of Baicalein and Galantamine (Ltf-BCL-GLM-lps) and evaluate their safety and efficacy by various in vitro and in vivo studies.

Methods: The liposomes (Ltf-BCL-GLM-lps) will be developed and optimized using the thin film hydration method, surface modified with lactoferrin, and characterized for particle size, zeta potential, morphological characteristics, entrapment efficacy, and stability studies. In vitro studies will be conducted using appsw239t and SH-SY5Y cell lines to assess cell viability, cellular uptake, enzyme inhibition, and biochemical analysis. In vivo studies to evaluate the pharmacodynamics and pharmacokinetics will be done in transgenic models of Drosophila and A β ₁₋₄₂-induced Alzheimer's rat models.

Results: The preliminary *in-silico* work has been completed, and the results demonstrate that Baicalein has a good binding affinity to BACE1, GSK-3 β , and Galantamine to α 7 nachrs. An extensive literature review was conducted to provide a comprehensive understanding of the background information. The methodology developed was carefully designed to meet the project's objectives.

Conclusion: The lactoferrin-functionalized liposomes loaded with Baicalein and Galantamine offer a promising therapeutic strategy to halt neurodegeneration in AD. It might prove to be an effective target for multiple pathways involved in neurodegeneration, paving the way for better treatment outcomes and improved patient quality of life.

Keywords: Alzheimer's Disease, liposomal drug delivery, neuroprotection, Baicalein, Galantamine



PD-DB-077: Detection of Asbestos in Talc-containing cosmetic products

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Asbestos is commonly referred to as a group of naturally occurring minerals and is harmful human carcinogen. Even a small amount of asbestos exposure is not safe for humans. Its concern is rising as asbestos is found to be present in talc-containing cosmetic products. Talc is a common ingredient in many cosmetic products like eye lashes, blushes and many more. Both talc and asbestos are silicate minerals that occur in the Earth's crust in close proximity, due to which talc is contaminated with some amount of asbestos. It is a known carcinogen which causes mesothelioma, lung cancer and other asbestos-related diseases. Talc-containing cosmetics are usually tested for the presence of asbestos. The presence of asbestos in cosmetic products has led to its recall as well as warnings from the FDA. Many methods are used to detect asbestos in cosmetics, such as Polarized light microscopy (PLM) and Transmission electron microscopy (TEM). The detection is based on optical, elemental and structural properties. Regarding the latter, these methods have their own drawbacks. Recently, AI techniques have also been used to detect asbestos in cosmetic products. Machine learning algorithms are used to analyse the images produced in microscopy for their accurate and speedy detection. It can be concluded that asbestos can be detected using traditional as well as AI techniques. Due to its harmful effects, the USFDA has proposed standardised methods to detect asbestos in cosmetics, especially in talc-containing cosmetic products.

Keywords: Asbestos, carcinogen, detection, AI machine algorithms



PD-DB-078: Printing Precision: E-Jet Fabricated Resveratrol Carriers for Local Breast Cancer Management

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Breast cancer is more than a disease – it's a silent force that alters bodies, burden lives. One in every eight women is affected globally. Despite many advancements in oncology, traditional chemotherapy continues to operate like a double-edged sword – as it targets cancer cell, it simultaneously exposes healthy tissues to toxic effects, often resulting in hair loss, fatigue, immune suppression and a severely compromised quality of life. There is a clear need for therapies that are not only effective but also kind. A biodegradable implant system engineered to deliver targeted therapy directly to the tumor site is introduced, thereby minimizing systemic toxicity and enhancing therapeutic precision. This is achieved by utilizing ELECTROHYDRODYNAMIC JET (E-JET) 3D PRINTING, a highly advanced microfabrication technique, the system allows precise deposition of drug loaded polymers with customizable structures and drug – release kinetics. Resveratrol which a plant-derived polyphenolic compound known for its anticancer, anti-inflammatory and antioxidant properties. However, Resveratrol has extremely poor bioavailability greatly limiting its therapeutic potential when administered orally or systemically. To overcome these limitations, Resveratrol is encapsulated within biocompatible biodegradable polymers such as poly PLGA or PCL. Through E-jet 3D printing, this combination allows the construction of customized implant with precisely controlled drug loading, porosity and degradation rate leading to sustained, localized drug release directly at the tumor site. This approach bypasses 1st pass metabolism and enhances local drug retention thereby significantly improving Resveratrol's bioavailability and therapeutic efficacy. By observing on-going in-vitro evaluations which included drug release profiling, cytotoxicity assays and biocompatibility testing with breast cancer cell lines. Additionally, the modular design of the implant provides opportunities for further enhancements, including co-delivery of imaging markers for real-time monitoring – bringing us closer to personalized cancer care. This not only addresses the limitations of conventional breast cancer therapies but also provides a versatile platform that combines the precision of E-jet 3d printing with the therapeutic promise of Resveratrol. By overcoming the compound's poor bioavailability through localized, sustained delivery, more effective alternative to systemic chemotherapy. With its potential for customization, co-delivery this approach marks a significant advancement in personalized, minimally invasive cancer care – ushering in a future where treatment is not only targeted but also truly patient-centered.



PD-DB-079: The Next Generation Prospects, Challenges, and Instability Countermeasures for Space Medicine.

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Background: NASA has reported that the medication onboard the spaceflight decreased therapeutic efficacy, as some of the drug products are degraded more rapidly due to exposure to the space environment, resulting in less effective medication. The studies conducted in the ISS have some limitations, as the reports of each design remain inconclusive. J.F.Reichard et al found that the degradation rate was very fast compared to the original manufacturer's packaging material, due to prolonged exposure to atmospheric conditions like secondary particle radiation, CO₂, O₂, and humidity. So, this project aims to investigate the space-simulated stability assessment of marketed available drug products for the Gaganauts. This investigation places us in a strong position to strategically select the most suitable drug product for both short and long-duration space missions.

Aims & Objectives: This project aims to investigate the instability caused by the space environment of the drug substance. To evaluate drug substances in ground-based simulation studies and with a real-time Nanosatellite monitoring system.

Methods: Simulating all the parameters of the space environment in the laboratory and collecting all the fingerprints using a non-destructive analysis method once this analysis has been completed. Then, the following drug substance has to be placed in the Nanosatellite. This Nanosatellite has been taken by the POEM vehicle in the PSLV rocket and put into the lower Earth orbital LEO. After that, the signals were transmitted from the Nanosatellite to the ground station for analysis in the chemometric software.

Results: All the components and subsystems have been manufactured for the nanosatellite. Still, the validation for the sensor has to be performed.

Conclusion: Predicting how microgravity might affect the physical and chemical properties of medications. Developing specialized packaging to protect medications from radiation, temperature variations, and other space-specific environmental factors. Researching alternative drug delivery methods that might be more suitable for space travel.

Keywords: Astronaut, Microgravity, Pharmacokinetics, Stability, Ionizing radiation.



PD-DB-080: A novel nano co-crystal strategy to enhance the dissolution and oral bioavailability of a poorly soluble drug using various coformers

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Background: Curcumin has been identified as a potential molecule for the treatment of TB and multi-drug-resistant TB though its ability to induce autophagy in non-infected and TB infected macrophages, and promotes the clearance of the bacteria through immune modulation. Cocrystallization is the technique which helps to solubilize the poorly soluble API in a manner similar to high energy solids and have a crystalline nature which shows higher stability despite only involving non-bonding interactions. This implies that cocrystals can be used to improve solubility in addition to increasing the stability of the API without altering the pharmacological properties of the drug. The modification of an existing coformer to improve the functional groups is a novel and unexplored concept. This approach can eventually lead to tailoring of coformers to suit the requirements of an API prior to cocrystallization.

Aims & Objectives:

Aim: The aim of the study is to formulate and evaluate the curcumin nano-cocrystals loaded Nanostructured Lipid Carriers to enhance bioavailability in the treatment of tuberculosis.

Objective: To identify and modify a suitable coformer. To synthesize and characterize the cocrystals of curcumin using the selected coformer. To formulate and characterize the Nanostructured Lipid Carriers containing cocrystals of curcumin. To perform in vitro studies to determine cytotoxicity, hemolysis and in vitro macrophage based study (Anti-TB activity). To perform the in vivo bioavailability (pharmacokinetic study).

Methods: Nicotinamide was chosen as the coformer due to its small size and modifiable group. It has one hydrogen bond donor and two acceptors. ADMET analysis was used to assess solubility and bonding potential of conjugates. Based on results, 2,4,6-trihydroxybenzaldehyde was selected. Reaction conditions were optimized for conjugation. The coformer was synthesized using imine formation reaction. This coformer was used for the synthesis of cocrystals and nanosized using top-down method. Cocrystals were characterized using PXRD, DSC, XRD, SEM, TGA, PLM, single crystal analysis, water wettability, and solubility studies. Nanostructured lipid carriers were evaluated for zeta potential, particle size, entrapment efficiency, drug loading, and stability. In-vitro studies included cocrystal dissolution, cytotoxicity, hemolysis, and macrophage-based anti-TB activity. In vivo bioavailability was conducted on mice.

Results: FTIR analysis confirmed coformer modification by showing a broadened N-H stretching band around $3180-3300\text{ cm}^{-1}$, in contrast to pure nicotinamide. This broadening is likely due to the presence of additional -OH groups, which absorb in a similar spectral region.

Conclusion: The study successfully demonstrated a novel approach of modifying a coformer to enhance its compatibility with curcumin, enabling effective cocrystallization. The resulting curcumin cocrystals, when incorporated into nanostructured lipid carriers, exhibited improved solubility, stability, and bioavailability. In-vitro and in-vivo evaluations confirmed the



enhanced pharmacokinetic profile and anti-TB potential of the formulation, supporting its application in tuberculosis therapy.

Keywords: Curcumin, coformer, coformer modification, Improved Bioavailability, Anti-TB activity.



PD-DB-081: Trojan Horse Strategies: Overcoming Blood-Brain Barrier Challenges for Neurodegenerative Diseases

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Background: The blood-brain barrier (BBB) acts as a hurdle by preventing the transport of therapeutic drugs into the brain restricting treatment of neurodegenerative disorders, namely, Alzheimer's and Parkinson's. These disorders cannot be cured by conventional drug delivery methods such as oral and intravenous routes as they fail to traverse the BBB. The Trojan Horse method disguises biologics as substances naturally crossing the barrier, improving the therapeutic outcomes.

Aims & objectives: To assess the efficacy, safety, and potential of the Trojan horse strategy while evaluating its patient outcomes and treatment adherence.

Methods: The Trojan horse leverages the method of Receptor Mediated Transcytosis (RMT), via endocytosis and transcytosis. The key types of study include antibody-receptor fusion proteins (e.g. TfR conjugates), exosome/vesicle-based delivery (e.g. RVG-Exosomes) and receptor-mediated peptide transport (e.g. Angiopep-2). The clinically engineered AAV gene therapy is deployed for targeted delivery in the in vitro and in vivo models of neurodegenerative diseases.

Results: Preclinical data from RMT-based Trojan horse enhance brain uptake up to 12-fold. Antibody fusion proteins that delivered "brainrestor", an anti-inflammatory agent, helped to achieve therapeutic concentrations in target glial cells. Also, the exosome based systems that delivered therapeutic micRNAs to substantia nigra neurons have led to 40% reduction in α -synuclein aggregation in Parkinson's models. This result validates the broad therapeutic potential for diverse modalities.

Conclusion: A novel approach is offered by the Trojan Horse method for bypassing the BBB in neurodegenerative diseases. This enables the delivery of a wider range of therapeutic molecules compared to other methods. While insufficient targeting specificity remains an impediment, surface functionalization with specific ligands can refine its delivery. This approach has a key potential for optimised CNS therapeutic delivery.

Keywords: Blood-brain barrier, Trojan Horse, Receptor Mediated Transcytosis, exosome, AAV gene therapy, neurodegenerative disorders



PD-DB-082: Targeting the Fat Vasculature: A Paradigm Shift in Anti-Obesity Therapeutics

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Obesity is a complex metabolic disorder characterized by excessive adipose tissue expansion, which relies heavily on vascular support not only for tissue growth but also for modulating adipocyte function and systemic energy balance. Targeting adipose vasculature thus offers a promising strategy to therapeutically reprogram fat metabolism at its origin. This study explores a vascular-targeted nanotherapeutic approach designed to induce angiogenesis-driven browning of white adipose tissue (WAT) into metabolically active brown-like adipose tissue (BAT), thereby enhancing energy expenditure and mitigating weight gain. Biodegradable PLGA-PEG nanoparticles were engineered and functionalized with adipose vasculature-targeting ligands—irgd and prohibitin-binding peptides—for selective WAT delivery. These nanocarriers encapsulated either rosiglitazone (a ppar γ agonist) or a prostaglandin E₂ analog, both of which are known to promote angiogenesis and browning. In vitro treatment of stromal vascular fractions (SVF) derived from inguinal WAT revealed upregulated expression of angiogenic markers (VEGF, integrins) and browning genes (UCP1, PGC-1 α). In vivo, intravenous administration of these formulations to diet-induced obese (DIO) mice over two weeks resulted in preferential nanoparticle accumulation in WAT vasculature, significant reductions in body weight gain, improved metabolic parameters (lowered insulin, triglyceride, and cholesterol levels), and increased WAT vascularization with histological evidence of browning. These findings support a novel vasculature-targeted nanotherapy as a transformative approach for obesity, shifting the paradigm from generalized weight loss to precise metabolic reprogramming via adipose tissue vasculature modulation.

Keywords: Adipose vasculature, obesity, nanotherapy, angiogenesis, targeted delivery, WAT browning, metabolic reprogramming



PD-DB-083: Formulation and Evaluation of Enteric-Coated Lansoprazole-Loaded Solid Lipid Nanoparticles (slns) for Controlled Drug Release

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Background: Lansoprazole, a proton pump inhibitor (PPI), is widely used for the treatment of acid-related gastrointestinal disorders, such as peptic ulcers and gastroesophageal reflux disease (GERD). However, its acid-labile nature and poor aqueous solubility limit its bioavailability and therapeutic efficacy. To overcome these limitations, Solid Lipid Nanoparticles (slns) offer a promising drug delivery system by enhancing drug stability, bioavailability, and controlled release. Furthermore, enteric coating ensures site-specific drug release in the intestine, preventing premature degradation in gastric pH.

Objective: The present study aims to formulate and evaluate lansoprazole-loaded slns with an outer enteric coating layer to achieve controlled and targeted drug release in the intestinal environment.

Methodology: Lansoprazole-loaded slns were prepared by the hot homogenization followed by ultrasonication method using stearic acid as lipid and Poloxamer 188 as stabilizer. A design of experiments (doe) approach was employed for optimization of formulation variables. The slns were then coated with an enteric polymer (Eudragit L100) using a fluidized bed coating process. The prepared formulations were evaluated for particle size, zeta potential, encapsulation efficiency, in vitro drug release (simulated gastric and intestinal fluids), and stability studies.

Conclusion: Lansoprazole-loaded slns with enteric coating present a novel and effective approach for enhancing the stability and controlled intestinal release of lansoprazole. This dual delivery system holds significant potential for improving therapeutic outcomes and patient compliance in the management of acid-peptic disorders.

Keywords: Lansoprazole, Solid Lipid Nanoparticles, Enteric Coating, Controlled Release, Eudragit L100, Proton Pump Inhibitor



PD-DB-084: The Sonic Solution: Harnessing Ultrasound and Nanotechnology to Breach Biofilm Defenses

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What if bacterial cells didn't just grow—but strategized? Bacterial survival is not solely dependent on proliferation, but on a highly coordinated and adaptive strategy—biofilm formation. Biofilms are an arranged group of microorganisms living within an extracellular polymeric substance (EPS) matrix produced by them and are adhered to each other on living or non-living surfaces. Within this environment, encapsulated by biofilms, microbes exhibit altered metabolic states, phenotypic variation, emergence of persister cells – dormant and antibiotic tolerant variations, which are able to evade pharmacological and immunological clearance. Bacterial biofilms are an ever-growing concern for public health, featuring both inherited genetic resistance and a conferred innate tolerance to antibiotic therapies. Biofilms are implicated in 80% of chronic infections. The configuration of these biofilms acts as a physical and biochemical barrier, hindering the penetration of antibiotics, inactivating drugs via matrix bound enzymes, also facilitating horizontal gene transfer of resistance determinants. Consequently, there is a growing interest in novel methods of drug delivery. One such method is the use of acoustically activated microbubbles, which undergo volumetric oscillations and collapse upon exposure to an ultrasound field. This sonic solution harnesses mechanical energy of ultrasound waves to activate drug loaded nano bubble complexes. These complexes undergo oscillation or collapse, causing shear stress, capable of penetrating and dismantling biofilm's dense EPS matrix. These precision drug delivery vectors, enhance site specific release efficiency upon acoustic activation. Moreover allows for localized high-concentration delivery precisely within the biofilm. In conclusion, ultrasound-mediated nanoparticle systems offer a shift in paradigm of biofilm management. By combining the mechanical force of sound and molecular precision of nanomedicine, this technique addresses the challenges of antimicrobial penetration and resistance. This advancement holds the capability of transforming treatment of chronic infections – from surgical wounds to cystic fibrosis lungs into a process that is targeted, effective and systematically safe.

Keywords: Biofilms, Drug delivery, Ultrasound, Nanotechnology



PD-DB-085: Neurocosmetics: a convergent path of neuroscience and skincare for targeted cosmetic interventions

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Neurocosmetics is an innovative and rapidly evolving interdisciplinary field that merges neuroscience with cosmetic science to develop formulations that influence the skin through neurochemical pathways. The skin, often described as a neuroendocrine organ, communicates bidirectionally with the central nervous system via neurotransmitters (acetylcholine, serotonin), neuropeptides (Substance P, CGRP), and specialized neuroendocrine cells such as Merkel and Langerhans cells. These components regulate skin homeostasis, inflammation, hydration, pigmentation, and aging. This review explores key neuroactive compounds—such as acetyl hexapeptide-8, niacinamide, cannabidiol, and GHK-Cu—that modulate neuro-signalling pathways to deliver clinical benefits in anti-aging, barrier repair, and skin tone regulation. Advanced delivery technologies including liposomal encapsulation, microneedle arrays, iontophoresis, and pH-responsive nanocarriers have enhanced bioavailability and skin penetration of these agents. Clinical data demonstrate significant efficacy: 27% reduction in wrinkle depth, 18% improvement in skin elasticity, and 45% decrease in rosacea-associated erythema. The review also addresses emerging research areas such as AI-guided personalized neurocosmetics, the gut-brain-skin axis, chrono cosmetic alignment with circadian rhythms, and bioelectronic skin stimulation. Additionally, it highlights regulatory ambiguities between cosmetic and therapeutic classifications and emphasizes the need for long-term safety evaluations. As consumer demand shifts toward functional and personalized skincare, neurocosmetics represents a transformative shift in dermatological innovation—bridging science and self-care to deliver both therapeutic and aesthetic outcomes.

Keywords: Neurocosmetics, Skin-brain axis, Neuropeptides, Neurotransmitter modulators, Smart delivery systems, Personalized dermatology.



PD-DB-086: Bridging Traditional and Precision Skincare Through Skinomics and Systems Biology

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Background: Historically, skincare has depended on broad strategies based on product development motivated by efficacy and subjective skin type categorization. However, more sophisticated methods are required due to the increasing complexity of skin biology and customer need for customized solutions. A comprehensive understanding of the molecular and cellular landscape of the skin is made possible by skinomics, which combines systems biology with genomic, proteomic, metabolomic, and microbiomic investigations. Precision skincare, in which formulations and treatments are customized to each person's own biological skin profile, is being made possible by this technological advancement.

Aim & Objectives: The purpose of this study is to investigate how traditional, efficacy-based skincare becomes precision skincare through the integration of skinomics and systems biology. Objectives include:

- Understanding the main systems biology and omics technologies causing this change.
- To learn how customized skin profiling can enhance effectiveness, forecast skin reactions, and customize treatments.
- To learn the implications on how precision skincare might affect consumer results and business procedures.

Methods and Results: Skinomics revolutionizes skincare personalization by integrating multi-omics profiling - genetics, proteomics, metabolomics, and microbiomics - to map each individual's unique skin biology far beyond traditional skin typing. By identifying precise biomarkers linked to conditions like sensitivity, pigmentation, aging and inflammation, skinomics uncovers the molecular mechanisms behind skin barrier

Function and other key processes. Advanced systems biology models use this deep data to predict how a person's skin will respond to specific ingredients and environmental factors, guiding truly customized formulations that maximize effectiveness and minimize irritation. Unlike static regimens, skinomics enables dynamic, adaptive care by continuously adjusting recommendations as biological and lifestyle factors change over time. This scientific, predictive, and responsive approach empowers consumers with tailored solutions, enhances treatment outcomes, drives brand trust, and bridges the gap between cosmetic skincare and personalized dermatological science.

Conclusion: The synergy of skinomics and systems biology marks a significant paradigm shift from generic to personalized skincare. Precision cosmetics, powered by data-driven insights, has the potential to revolutionize skin health management by delivering scientifically tailored, safer, and more effective skincare solutions aligned with individual needs.

Keywords: Precision skincare, skinomics, systems biology, personalized cosmetics, multi-omics, skin profiling, dermatology, microbiome, genomics, metabolomics



PD-DB-087:AI-Driven Design Of Lipid Nanoparticles For Targeted Neurological mrna Therapies

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To unlock the promise of mrna-based treatments, it is essential to widen the range of lipid nanoparticle (LNP) availability. Lipid nanoparticles have emerged as a reliable vehicle for mrna delivery, as demonstrated by the success of COVID-19 vaccines. A key gridlock in lipid nanoparticle development is in finding new ionizable lipids. Ionizable lipids are conventionally developed through costly trial-and-error experiments that aren't always efficient. In this study, we employ artificial intelligence (AI) to develop targeted lnp's that can cross the blood-brain barrier for neurological diseases such as Parkinson's or Alzheimer's, delivering mrna to restore and modulate neuronal functions by predicting two LNP parameters: apparent pka and mrna delivery efficiency. The developed lnp's combined with high-throughput patient data were virtually screened, synthesised and tested in lab-grown organoids and refined iteratively. This continuous refinement through iteration delivered promising results. This approach streamlines the design and evaluation of diverse ionizable lipid libraries, accelerating the development of lnp's for targeted and efficient mrna delivery. The AI model is reliable in structure-activity relationship studies.

Keywords: ionizable lipids, mrna delivery, virtual screening, structure-activity relationship, Parkinson's disease, Alzheimer's disease.



PD-DB-088: Advancing Therapeutics Through Lipid Nanoparticles: Bridging Science and Patient Care

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Background: Pharmaceutical sciences are bridging gaps between patient care and science with the help of innovative drug development. How intensively a private company invests in research and development depends on the public sector investment in basic biomedical research and development.

Aims and objectives: To take a look at how lipid based nanosystems are transforming drug delivery by reducing adverse effects, transforming drug delivery and enabling personalised medicine. This paper focuses on the role of nanotechnology in overcoming targeted drug delivery challenges and providing better patient outcomes.

Methods: One of the major challenges in modern therapeutics is the efficient delivery of active pharmaceutical ingredients to the target site; this can be overcome by controlling drug delivery. Recent developments have shown that nanoparticles are great as drug carriers. Introducing a safe and effective nanotechnology-based delivery system and improving the stability of mRNA is needed for the successful mRNA treatment. Nanotechnology has enabled customized drug delivery, especially in oncology. Success in delivering hydrophobic and hydrophilic therapeutics can be seen because of lipid-based nanoparticles such as liposomes, solid lipid nanoparticles, and nanostructured lipid carriers.

Result: Nanoparticles reduce systemic toxicity by delivering drugs to tumor cells directly as well as provide protection to mRNA from extracellular degradation hence improving the efficacy. Drugs are also prevented from rapid degradation and hence lower doses of drugs would be required.

Conclusion: Through the modern innovations seen in nanotechnology-based drug delivery systems, personalised medicines, pharmacogenomic therapy and many more not only does science foster but it improves the quality of life of patients through lowered hospital stays and lesser long-term expenses as well as growth in the research and development sector.

Keywords: Lipid nanoparticles, solid lipid nanoparticles (SLN), nanostructured lipid carriers (NLC), liposomes, hydrophobic therapeutics, hydrophilic therapeutics, drug delivery systems.



PD-DB-089: Overcoming Therapeutic Barriers in Bone Cancer: A Systematic Review of Drug Delivery Innovations Targeting Multidrug Resistance

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Background: Multidrug resistance remains a major barrier in treating bone cancers, particularly osteosarcoma. Mechanisms like P-glycoprotein (P-gp) overexpression, acidic tumour microenvironments, and premature drug degradation reduce drug efficacy. Conventional chemotherapeutics often fail to bypass these resistance pathways, demanding novel delivery approaches that can modulate pharmacokinetics and intracellular targeting.

Aim & Objective: To critically evaluate and synthesize innovative drug delivery strategies that overcome multidrug resistance (MDR) in bone cancer—specifically targeting efflux pump inhibition, pH-sensitive release, and nanoparticle-based formulations—to enhance intracellular drug accumulation and therapeutic outcomes.

Methods: A systematic literature review was conducted in accordance with PRISMA guidelines using databases such as pubmed, Cancer Drug Resistance, BMC, and sciencedirect, covering publications from January 2012 to March 2025. The search focused on peer-reviewed studies related to multidrug resistance (MDR) in bone cancer, specifically addressing efflux pump inhibitors, pH-sensitive carriers, or nanoparticle-based drug delivery in in vitro, in vivo, or preclinical models. Only English-language articles were considered. From 1,342 initial records, 312 duplicates were removed. After screening 1,030 articles, 874 were excluded. Of 156 full texts assessed, 143 were excluded due to irrelevance, lack of experimental data, or absence of the specified delivery approaches. Ultimately, 13 studies were included in the final review.

Results: Efflux pump inhibitors (e.g., tariquidar, elacridar) enhanced intracellular drug retention by 2.5–4.2-fold. pH-sensitive delivery systems exhibited up to 80% release at tumour-relevant pH (6.5), improving site-specific action. Engineered nanocarriers such as pegylated liposomes and mesoporous silica nanoparticles increased drug bioavailability by 3–6-fold while reducing systemic toxicity.

Conclusion:

Strategic modulation of drug delivery mechanisms—via efflux pump inhibition, pH-triggered systems, and functionalized nanoparticles—holds transformative potential in overcoming MDR in bone cancer, leading to enhanced therapeutic outcomes and minimized adverse effects.

Keywords:

Bone cancer, Multidrug resistance, Drug delivery, Efflux pump inhibitors, pH-sensitive systems, Nanoparticles, Targeted therapy.



PD-DB-090: Pharmacokinetic and Clinical Relevance of the Medoxomil Moiety in Olmesartan: A Scoping Review

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Background: Medoxomil is a pharmacologically inert promoietty used in the synthesis of several prodrugs, most notably olmesartan medoxomil—an angiotensin II receptor blocker (ARB) indicated for hypertension. Its utility lies in enhancing the oral bioavailability of poorly absorbed parent drugs by increasing lipophilicity and enabling transporter-mediated uptake. After oral administration, olmesartan medoxomil undergoes rapid enzymatic hydrolysis to release active olmesartan. This review synthesizes current evidence regarding the pharmacokinetics, metabolism, and clinical implications of the medoxomil moiety in olmesartan formulations.

Methods: A scoping review was conducted using literature published from 2000 to 2025 across pubmed, Scopus, and regulatory sources. Search terms included “olmesartan medoxomil,” “medoxomil prodrug,” “carboxymethylenebutenolidase (CMBL),” and “bioavailability.” Inclusion criteria encompassed original pharmacokinetic studies, clinical trials, formulation studies, and pharmacovigilance data pertaining to the medoxomil moiety’s absorption, metabolism, or clinical relevance.

Results: Olmesartan medoxomil is enzymatically hydrolyzed in the proximal small intestine primarily by CMBL, with minor roles from paraoxonase-1 and chemical hydrolysis. The intact prodrug is undetectable systemically, and the medoxomil group is rapidly degraded into non-toxic metabolites. The absolute bioavailability of olmesartan is ~26%, with a T_{max} of 1–2 hours. The prodrug facilitates OATP2B1-mediated uptake, improving systemic exposure. Bile acid sequestrants and OATP2B1 inhibitors can impair absorption, while food has minimal effect. Novel delivery systems such as nanocrystals and Self-Microemulsifying Drug Delivery System (SMEDDS) have demonstrated enhanced absorption in preclinical studies. No significant safety or pharmacological concerns have been identified for the medoxomil moiety in recent pharmacovigilance reports.

Conclusion: The medoxomil moiety is essential for the pharmacological success of olmesartan by enabling effective gastrointestinal absorption and systemic availability of the active drug. Its rapid and complete hydrolysis, coupled with lack of systemic exposure or toxicity, highlights its value as a safe and effective prodrug strategy. In special populations, including pediatrics, and malnourished individuals, variability in hydrolytic enzyme expression may necessitate tailored dosing. Clinicians should consider timing of administration with interacting agents, but overall, the medoxomil-based design of olmesartan remains a clinically sound and biopharmaceutically rational approach

Key Word: Medoxomil



PD-DB-091: Polymorphism in Pharmaceuticals: Unlocking the Secrets of Solid-State Science

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Background: Polymorphism is a phenomenon where a compound exists in more than one crystalline form, plays a major role in the physical and chemical properties of drug candidates. The polymorphic form can have a great effect on solubility, stability, melting point, and bioavailability. All these properties affect a drug's therapeutic profile and ultimately its manufacturability.

Aims & Objectives: This review seeks to address the profound effects polymorphism- as well as solid-state characterization, can have during the pharmaceutical development process. The intention is to explore the effects that polymorphic forms can have on drug quality, as well as evaluation methods which can assist with the differentiation and characterization of polymorphs.

Methods: We report on a comprehensive review of the literature and case studies on solid-state characterization from thirty published studies. Pages particular to the methods section are constructed to include the solid-state characterization techniques of Differential Scanning Calorimetry (DSC), Powder X-Ray Diffraction (PXRD), Hot Stage Microscopy, Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and Thermogravimetric Analysis (TGA).

Results: Case studies are presented to include the studies of rifampicin, ranitidine, and indapamide, which show that polymorphic forms depend generally on thermal properties related to their solubility and stability. Solid-state characterization methods can be employed reliably, to confirm and differentiate polymorphic forms, which can provide the basic tenets necessary to develop optimized formulations.

Conclusion: Polymorphism is an integral component of research pertaining the development of effective and stable drug products. Solid-state characterization methods can facilitate an informed decision pertaining to the polymorphic form when first developing a drug product enabling consistency in therapeutics and subsequent regulatory applications.

Keywords: Polymorphism, Solid-state characterization, Solubility of drugs



PD-DB-092: Transition from Injection to Pill: Advanced Delivery Strategies for GLP-1 Receptor Agonists

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GLP-1 receptor agonists (GLP-1 ras) serve as effective treatments for Type 2 Diabetes, obesity and demonstrates growing benefits for cardiovascular, renal and hepatic diseases. Currently, GLP-1 ras are predominantly administered via the subcutaneous route, which is a burden for patients having chronic conditions. Studies have shown that 82% of patients prefer once a day oral medication over injection treatments. This high demand for oral medications represents both an unmet medical need and a massive market potential since GLP-1 ras are projected to reach hundreds of billions of dollars in sales by 2035. For this, various strategies have been implemented. Permeation enhancers such as salcaprozate sodium (SNAC) have been used in oral semaglutide Rybelsus®, which protects the peptide from low pH of gastric acid and promotes its transport through the membrane. Peptide stapling is a new technique that aims to improve the permeability and stability of peptides and thus remains as an area of active research interest. Small-molecule GLP-1 ras, such as Eli Lilly's orforglipron, Viking Therapeutics' VK2735, and Roche's CT-996, have shown promising therapeutic activity. The aim of this article is to present various methods utilized to increase the oral bioavailability of GLP-1 ras. Our objective is to understand the role of new permeation enhancers, analyze the peptide stapling approach, and assess the current status of oral GLP-1 ras. This shift towards oral administration of GLP-1 ras is intended to significantly increase patient compliance, expand market accessibility, and redefine the treatment of chronic metabolic diseases.

Keywords:

GLP-1 Receptor Agonist, Oral Bioavailability, Permeation Enhancers, Peptide Stapling, Semaglutide, Orforglipron, Drug Delivery



PD-DB-093: Crossing the Blood–Brain Barrier: Advances and Limitations of Nanoparticle Drug Delivery for CNS Disorders

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Background: The blood-brain barrier (BBB) presents considerable challenges for the pharmacological treatment of central nervous system (CNS) disorders by blocking more than 98% of small molecules [4] and almost all biologics. Currently, Alzheimer's disease, glioblastoma, Parkinson's disease, and epilepsy remain inadequately treated by therapies available today. Because of enhanced targeting and improved biocompatibility and bioavailability, nanoparticle-based systems can potentially overcome the BBB-associated drug delivery problems revolutionarily.

Aims & Objectives: This review focuses on Alzheimer's, glioblastoma, Parkinson's, and epilepsy, critically examining the advances in nanoparticle-mediated BBB crossing or using these diseases as the focus and the translational and regulatory barriers to clinical application.

Methods: The databases pubmed, Scopus, and sciencedirect were searched for peer-reviewed published articles dated between 2013 and 2025. The listed categories of nanocarriers included lipid nanoparticles (lnps), polymeric nanoparticles, exosomes, dendrimers, and magnetic nanoparticles. The transport mechanisms studied were receptor-mediated transcytosis, adsorptive-mediated uptake, and magnetic targeting.

Results: Transferrin-tagged systems and insulin receptor targeting formulations are examples of functionalized nanoparticles that have shown improved CNS delivery in preclinical glioblastoma and Alzheimer models [2][5]. Externally guided magnetic nanoparticles have shown the ability to penetrate the BBB and demonstrated spatial control of CNS targeting. Some of the most important challenges include unanticipated protein corona formation, immune system removal, low escape from endosomes, and limited scalability.

Conclusion: Even though approaches built on nanoparticles mark a radical change in the delivery of drugs to the central nervous system (CNS), their clinical use is limited by the sphere of life science and technology complexities, as well as production hurdles. Areas of greater focus and advances should include the combination of intelligent technologies, biomimetic, and magnetism-based systems, tailored to specific diseases.

Keywords: Blood–brain barrier, Nanoparticles, Magnetic nanoparticles, CNS drug delivery, Alzheimer's disease, Glioblastoma, Parkinson's disease, Epilepsy, Receptor-mediated transport, Translational barriers.



PD-DB-094: Advances in Nanocrystal Technology for Drug Delivery Overcoming Poor Solubility and Bioavailability in Modern Pharmaceuticals

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Nanocrystals have revolutionized the field of pharmaceutical drug delivery, offering promising solutions for medications that exhibit poor water solubility. These particles, composed entirely of the active drug substance and typically sized between 10 and 1000 nanometers, are particularly effective in addressing the challenge of low oral bioavailability—a limitation that affects a substantial proportion of both marketed drugs and compounds in the development pipeline. The reduction in particle size leads to a significant increase in surface area, which in turn enhances the dissolution rate and apparent solubility of the drug, as described by fundamental physical principles such as the Noyes-Whitney and Ostwald-Freundlich equations. Unlike many other nanoparticle-based delivery systems, nanocrystals do not require additional carriers or excipients, allowing for higher drug loading and efficient administration, especially for high-dose therapies. Nanocrystals can be produced using either top-down approaches, such as media milling and high-pressure homogenization, or bottom-up methods like precipitation and supercritical fluid processing. Each technique offers specific advantages and challenges in terms of scalability, stability, and particle size control. The successful commercialization of nanocrystal-based formulations, including sirolimus, aprepitant, and fenofibrate, demonstrates their clinical viability. Beyond improving solubility and absorption, nanocrystals also present opportunities for targeted drug delivery, controlled release, and alternative administration routes such as transdermal or pulmonary delivery. Ongoing research is dedicated to refining production techniques and expanding the therapeutic applications of nanocrystals, positioning them as a vital technology in modern drug development.

Keywords: Spray-dried liposomes, unloaded liposomes, phosphatidylcholine, cholesterol, nanocarrier, controlled release, qbd, trehalose, atorvastatin, drug delivery.



PD-DB-095: Gliptins and the Blood-Brain Barrier: Overcoming the challenges faced by type 2 diabetic drugs repurposed for “Type 3 Diabetes” through targeted drug delivery
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Background:

Alzheimer's hallmarks include neuronal loss, intracellular neurofibrillary tangles of hyperphosphorylated tau aggregates and extracellular beta-amyloid plaques. Alzheimer's shares multiple pathophysiological mechanisms with type 2 diabetes such as insulin resistance, impaired insulin signaling, oxidative stress, and advanced glycosylation end products, resulting in the characterization of Alzheimer's as “type 3 diabetes”. This sets the basis for utilizing these commonalities to repurpose related drugs. Gliptin class of antidiabetic drugs increase insulin secretion by proteolytic enzyme DPP-4's inhibition. Their therapeutic implementation for Alzheimer's is severely limited by their inability to cross the blood-brain barrier (BBB), marking it as the primary bottleneck, as even partial permeability requires potentially toxic initial concentrations.

Aims & Objectives: Examine the viability of gliptins in Alzheimer's treatments. Analyse and evaluate various BBB-targeted delivery methods for gliptins.

Methods: A structured review was conducted using peer-reviewed studies from databases like Google Scholar, pubmed and Science Direct using relevant keywords.

Results: While several gliptins show promising indirect benefits to the brain, including decreasing beta-amyloid and phosphorylated tau levels [6], most failed to achieve the therapeutic concentration on their own due to their size, restricted pinocytosis, efflux transporters and metabolic enzymes. Those that succeeded were characterized by low molecular weight and high lipophilicity. Drug delivery methods such as intranasal chitosan-loaded nanoparticles, Yeast-wall vesicles, showed increased cerebral concentrations, but such methods are rare and are severely lacking in translational implementation, highlighting significant research gaps for future studies.

Conclusion: Repurposing gliptins for Alzheimer's can lead to more resource effective options. These inhibitors face the drawbacks of low BBB permeability, lack of clinical trials and much needed research on delivery and optimization. New innovative nanocarrier and intranasal delivery methods seek to bridge that gap. While yet to start clinical trials, it has now shifted the problem from overcoming a specific complex disease to the universal problem of drug delivery through the BBB.

Keywords: BBB, Gliptins, Alzheimer's disease, Targeted drug delivery, Drug repositioning.



PD-DB-096: Inject, Heal and Regenerate: Self-Healing Injectable Hydrogels in Tissue Recovery

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Background: Self-healing injectable hydrogels have become a ground-breaking class of biomaterials. These hydrogels, which are made to resemble the extracellular matrix, have the ability to change from a fluid state when sheared to a solid-like structure when injected, supporting minimally invasive treatments. They find use in tissue regeneration, wound healing, localized drug delivery as well as 3D bioprinting due to their exceptional capacity to regain their structure following deformation.

Aims & Objectives: Investigating the formation of smart hydrogels, evaluating their qualities and their benefits in treatment regimen is being explored. Understanding their special capacity for self-healing, their ease of injection is also understood.

Methods: To learn how such hydrogels are prepared through reversible bonds such as hydrogen bonding and metal coordination, a range of published research papers and case studies were examined and studied. Review was done on the methods by which rheometers were applied to test their strength and texture, as well as the ways they can be injected through very small needles without losing their gel composition. In order to determine how effective these hydrogels are when injected in living tissues, research involving animal models was reviewed.

Results: The results showed that these hydrogels effectively exhibited outstanding shear-thinning behavior and quick self-healing capabilities, guaranteeing smooth injectability. Improved wound closure rates, improved cardiac tissue recovery, and effective localized drug delivery were among the encouraging tissue regeneration results observed in in vivo models. These hydrogels also worked well as bioinks for extrusion-based 3D bioprinting, preserving structural integrity while promoting cell growth and viability.

Conclusion: Due to their multifunctional therapeutic effects, mechanical resilience, and injectability; self-healing injectable hydrogels have enormous potential in regenerative medicine. Standardizing rheological assessment procedures and converting preclinical success into clinical applications ought to be the main goals of future studies.

Keywords: Self-healing hydrogels, Injectable biomaterials, Tissue regeneration, Rheology, 3D bioprinting, Drug delivery



PD-DB-097: Nanotechnology and Cubosomes: A Review Article on Their Potential in Biomedical Sciences

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Background: Cubosomes are lipid-based nanoparticles with a bicontinuous cubic liquid crystalline structure, offering significant potential in drug delivery due to their structural versatility and high drug-loading capacity. These nanocarriers can encapsulate hydrophilic, lipophilic, and amphiphilic drugs, making them ideal for sustained and controlled drug release.

Aims & Objectives: The aim of this review is to explore the structural characteristics, preparation techniques, and therapeutic applications of cubosomes. Key objectives include:

- Understanding the structure and components of cubosomes
- Discussing preparation methods, including top-down and bottom-up approaches
- Examining therapeutic applications, such as oral, ophthalmic, topical, intravenous, intranasal, and pulmonary delivery

Methods: Cubosomes can be prepared using various methods, including

- Top-down approach: Using sonication and high-pressure homogenization to fragment bulk cubic phase gels
- Bottom-up approach: Using hydrotropes to lower energy inputs and facilitate self-assembly
- Dilution-based method: A type of bottom-up approach that produces cubosomes without requiring time-consuming fragmentation

Results: Cubosomes have shown promising results in various therapeutic applications, including:

- Sustained drug release: Cubosomes provide controlled release of drugs over time, improving efficacy and reducing side effects
- Bioadhesion: Their adhesive properties enable prolonged contact with biological membranes, enhancing drug absorption
- Protection from degradation: Cubosomes shield drugs from enzymatic and physical degradation, ensuring stability and bioavailability

Conclusion: Cubosomes represent a highly promising nanocarrier system for drug delivery, offering versatility, biocompatibility, and potential for surface functionalization. Their unique structural properties and ability to encapsulate various therapeutic agents make them suitable for diverse medical applications. Further research is needed to fully understand their characteristics and optimize their use in clinical settings.

Keywords: Cubosomes; Nanotechnology; Drug delivery; Biocompatibility



PD-DB-098: Exploring Novel Cyclosporine-A Formulations for Ocular Delivery

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Cyclosporine A (csa) formulations such as Restasis (Allergan Inc, USA, 2002) and Cequa (Sun Pharma, USA, 2018) are the mainstay treatment options for Keratoconjunctivitis sicca (KCS) or more commonly known as Dry Eye Syndrome (DES) which is characterized by loss of tear film homeostasis, hyperosmolarity, ocular surface inflammation and damage. Cyclosporine A exerts its immunomodulatory effects by inhibiting calcineurin receptors called cyclophilin, ultimately preventing T-cell infiltration, activation, and the subsequent release of inflammatory cytokines. It also has anti-apoptotic action, which protects the human conjunctival epithelial cells and improves goblet cell density. Although the safety and efficacy of Cyclosporine A has been well established for the treatment of DED, it poses several formulation challenges such as poor drug solubility, short pre-corneal residence time and poor patient compliance. Traditionally it has been formulated as oil-based solutions and emulsions for example Restasis® which was the first topical cyclosporine A formulation approved by FDA in 2003, a 0.05% oil in water ophthalmic emulsion of cyclosporine A which however has various drawbacks like low bioavailability, irritation, burning and blurred vision. Various delivery vehicles are also used in these homogenous emulsions such as glycerin (2.2%), castor oil (1.25%), polysorbate 80 (1%), carbomer co-polymer A (0.05%) etc. Hence, many clinical trials have been carried out worldwide to provide an alternative ocular delivery route to the existing oil-based formulations. Some notable advancements include; the development and testing of csa cyclodextrin-based ternary complex loaded dissolvable nano drug reservoir films in dry eye mouse models, and development of novel micellar eye drop formulation using octylphenol polyethylene glycol ether (OP-40), a surfactant with good delivery properties and polyoxyethylene hydrogenated castor oil (RH-40), a non-ionic surfactant which enhances stability. These major advancements offer a promising potential to provide quick and effective treatment for DED as well as alleviate patients from the adverse effects.



PD-DB-099: Advancing Cancer Immunotherapy: Lipid Nanoparticle-Based mrna and Gene Delivery Platforms

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Background: Messenger RNA (mrna)-based therapeutics represent a revolutionary approach in cancer immunotherapy, facilitating transient expression of critical antigens, cytokines, and immunomodulatory factors. Despite their potential, the inherent instability, immunogenicity, and inefficient delivery of mrna pose significant barriers to clinical efficacy. Lipid nanoparticles (lnps), validated through COVID-19 vaccines, have emerged as promising carriers to overcome these limitations.

Aims & Objectives: This review systematically evaluates the evolution and innovation in LNP platforms for mrna and gene-based cancer immunotherapies. It aims to highlight advancements in delivery efficiency, explore solutions for physiological barriers, assess stability, safety, and scalability concerns, and delineate future research trajectories for clinical translation.

Methods: A thorough review of literature encompassing preclinical and clinical research studies was conducted. Databases were comprehensively searched to identify key publications on physicochemical properties of lnps, cellular uptake, endosomal escape mechanisms, surface modifications, and manufacturing scalability.

Results: lnps have shown considerable progress in stabilizing mrna, enhancing cellular uptake, and improving specificity and endosomal escape efficiency. Surface engineering strategies, including ligand-based targeting of dendritic cells, significantly advanced therapeutic efficacy. Promising preclinical outcomes were observed in LNP-mediated CAR-T cell therapies, mrna vaccines, bispecific antibody delivery, and combination therapies. Scalable manufacturing techniques like microfluidics and tangential flow filtration, alongside enhanced storage protocols, further bolster clinical feasibility.

Conclusion: Addressing immunogenicity, refining targeting specificity, optimizing endosomal escape, and navigating regulatory landscapes are essential future directions to fully harness the therapeutic potential of LNP-based strategies.

Keywords: mrna therapeutics, lipid nanoparticles, cancer immunotherapy, endosomal escape, surface engineering, dendritic cell targeting, clinical translation.



PD-DB-100: Engineering Biomaterial Scaffolds for Melanoma: Innovations in 3D Printing and Nanoparticle-hydrogel scaffolds Enhanced Drug Delivery.

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The treatment of melanoma has been transformed by recent developments in biomaterial engineering, which combine 3D printing with nanoparticle-hydrogel scaffolds to improve tumor suppression, tissue regeneration, and medication delivery. Tumor heterogeneity, drug resistance, and immune evasion are problems for traditional therapy, such as immune checkpoint inhibitors and targeted medications. In response, biocompatible polymer-based 3D-printed scaffolds, like polylactic acid-fluorohydroxyapatite composites, provide structural support and regulated chemotherapeutic drug delivery. Hydrogel-based systems that are reinforced with flavanone@ZIF-8 nanoparticles, graphene oxide, and metal-organic frameworks aid in the healing of surgical wounds and enable antibacterial and anti-cancer treatment. Furthermore, bioactivity, extended drug release, and mechanical stability are enhanced by intelligent biomaterials such as tannic acid-modified scaffolds, polyhedral silsesquioxane nanoparticles, and hydrogels based on gelatin methacryloyl. New approaches concentrate on incorporating magneto-piezoelectric nanoparticles, which improve tumor elimination by boosting immune responses and biofilm destruction. Tumor-specific precision is provided by personalized medicine techniques such modified chimeric antigen receptor (CAR-T) therapies and melanoma-targeting polymer micelles. For flexible and patient-specific melanoma treatment, future studies should focus on bio fabrication methods that integrate 3D bioprinting, nanotechnology, and immune regulation. Notwithstanding encouraging outcomes, there are still issues with tumor targeting, scaffold degradation, and clinical translation. To overcome drug resistance and maximize therapeutic results in the treatment of melanoma, precision medicine will need to advance with biomaterials, real-time biosensing, and combination therapies.

Keywords: Melanoma, 3D-printed scaffolds, nanoparticle-embedded hydrogels scaffolds, photothermal therapy, nanotechnology, immune modulation, tissue engineering, precision medicine



PD-DB-101: Revolutionizing drug development: how ai and machine learning are shaping the future of medicine-a review

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Artificial Intelligence (AI) and Machine Learning (ML) are rapidly changing the way new medicines are discovered and developed. These technologies can process vast amounts of biomedical data, helping researchers identify drug targets faster, design better molecules, and predict how drugs will behave in the body—all in a fraction of the time and cost of traditional methods. Tools like alphafold have made major breakthroughs in understanding protein structures, while AI-based screening has led to the discovery of promising drug candidates within weeks instead of years. AI is also making clinical trials more efficient by identifying the right patients and predicting outcomes with high accuracy. While there are still challenges—such as ensuring data quality, making models understandable, and meeting regulatory standards—new approaches like explainable AI and federated learning are helping to overcome these barriers. Looking ahead, the integration of AI with emerging technologies like organ-on-a-chip systems, quantum computing, and 3D printing could revolutionize personalized medicine. This review explores how AI and ML are not just speeding up the drug development process, but also making it smarter, more precise, and more patient focused.



PD-DB-103: Design and evaluation of extracellular vesicles loaded with Doxorubicin and lycopene and its anticancer activity on lung Cancer cell line

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Objective: To develop and optimize lemon-derived extracellular vesicles (levs) for the co-delivery of Doxorubicin and lycopene to enhance anticancer activity against A549 lung cancer cells.

Methods: levs were isolated using 12% PEG-mediated precipitation. Drug loading was performed via passive incubation and optimized using Central Composite Design, with drug-to-EV ratio and incubation time as variables. Characterization included NTA, TEM, DLS, and zeta potential analysis. In vitro release, cytotoxicity (MTT, SRB), combination index, apoptosis (DNA fragmentation, AO/EB staining), and 3-month stability were evaluated.

Results: Optimized levs showed a size of 160.2 nm, PDI 0.289, and zeta potential -15.1 mv. Encapsulation efficiency was 76.45% Doxorubicin and 78.12% lycopene. Sustained drug release followed Korsmeyer-Peppas kinetics. Co-loaded levs exhibited superior cytotoxicity and synergistic effects versus free drugs. Apoptosis assays confirmed enhanced cell death. The formulation remained stable over 3 months.

Conclusion: levs are a stable, natural nanocarrier offering synergistic and sustained delivery of Doxorubicin and lycopene, showing promise for lung cancer therapy.

Keywords: Doxorubicin, Lycopene, Extracellular vesicles, NTA, MTT and Apoptosis.



PD-DB-104

3D Printed Polymeric Microneedles as Emerging Platforms for Targeted Drug Delivery in Therapeutic, Neurological and Cancer Applications

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Background: Microneedles (MNs) have gained immense attention as minimally invasive drug delivery platforms capable of bypassing the stratum corneum barrier. Among them, polymeric microneedles (PMNs) have emerged as promising vehicles due to their high drug-loading capacity, patient compliance, biodegradability, and cost-effectiveness. Recent advances in additive manufacturing, particularly three-dimensional (3D) printing, have revolutionized the design, precision, and functionality of PMNs, enabling tailored drug delivery for diverse biomedical applications.

Aims and Objectives: This study aims to explore the therapeutic and disease-specific applications of 3D-printed PMNs, with a focus on their potential in cognitive and cancer-based drug delivery. We further highlight how incorporation of nanomaterials enhances mechanical strength, controlled release, and therapeutic outcomes.

Methods: A comprehensive review of current fabrication strategies, including direct (stereolithography, fused deposition modeling, two-photon polymerization) and indirect (Solvent Casting, Mold-based printing) methods of 3D-printed PMNs, was undertaken. Applications were systematically categorized as therapy-based, disease-specific, neurological, and cancer-oriented.

Results: 3D-printed PMNs demonstrated versatility in delivering small molecules, peptides, proteins, hormones, and vaccines. Therapy-based uses include sustained analgesic and hormonal delivery, while disease-oriented applications range from insulin delivery for diabetes to topical treatment of dermatological disorders. Cognitive applications involve transdermal delivery of anti-Alzheimer's and antipsychotic drugs, whereas cancer-focused approaches include intratumoral chemotherapy, cancer vaccines, and combination therapies. Integration of nanomaterials further improved drug encapsulation efficiency, release kinetics, and reduced systemic toxicity, thus expanding their clinical potential.

Conclusion: 3D printing has transformed PMNs into customizable, patient-centric drug delivery systems with broad pharmaceutical relevance. Their ability to integrate advanced materials, achieve precision dosing, and target complex diseases underscores their role as next-generation therapeutic platforms.

Keywords: Polymeric microneedles, 3D printing, drug delivery, nanomaterials, cancer therapy, neurological disorders



PD-DB-105

From Data to Depot: The Role of Artificial Intelligence and Machine Learning in Long-Acting Injectable Development

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Background:

Long acting injectables have revolutionized the management of chronic diseases by enabling sustained drug release, improving adherence, and enhancing therapeutic outcomes. However, their development involves complex formulation and pharmacokinetic challenges. Artificial intelligence and machine learning are emerging as transformative tools in pharmaceutical research, offering data-driven approaches for formulation design, release profile prediction, and clinical outcome modeling.

Aims & Objectives:

To systematically evaluate current and emerging applications of artificial intelligence and machine learning in the development, optimization, and clinical utilization of long-acting injectables, with a focus on formulation strategies, PK/PD modeling, and patient outcomes.

Methods:

A narrative review was conducted by searching PubMed, ScienceDirect, and Google Scholar for articles from the past 10 years on AI and ML applications in drug delivery, focusing on long acting injectables. Key topics including formulation prediction, PK modeling, and real-world analytics were synthesized.

Results:

AI and ML have been applied to predict drug release kinetics from depot systems, optimize formulation parameters such as excipient ratios and particle size, and simulate pharmacokinetic profiles of long acting injectables. ML algorithms like artificial neural networks (ANNs), support vector machines (SVMs), and random forests have improved formulation development and in vitro–in vivo correlation (IVIVC). Furthermore, AI has enabled analysis of real-world data to monitor patient adherence and treatment response, especially in psychiatric and HIV LAI therapies.

Conclusion:

AI and ML offer powerful tools to streamline LAI formulation, enhance PK/PD modeling, and support clinical decisions. Their integration into regulatory and digital health systems could accelerate the development and adoption of next-generation LAIs.

Keywords:

Artificial Intelligence, Machine Learning, Long-Acting Injectables, Drug Delivery, Formulation Optimization

Category 2

Drug Regulatory Affairs and Pharmaceutical Management

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DRA-PM-001

Global Pharmacovigilance Synergy: Reimagining India's Role in Active–Passive Surveillance with Insights from the USA and EU

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The global pharmaceutical and medical device companies need to have real-time safety monitoring and rules that put patients first. The modification is based on two main pillars of safety monitoring: active and passive systems. Together, they make it clear what the dangers and advantages of pharmaceuticals and technology are once they have been approved. In older US and EU systems, structured frameworks, linked databases, and tech-enabled tools like electronic health records and patient registries have made it easier to find and fix problems. India's pharmacovigilance system is improving yet still struggling. For instance, it uses no real-world data for active monitoring, has unconnected reporting networks, and weak passive reporting models. In this essay, we'll take a look at the US, EU, and Indian safety monitoring systems. The essay explores the main differences between them in terms of structure, operation, and application. Topics covered include how these systems detect safety warnings, what the government is doing about it, and the roles played by manufacturers, healthcare providers, and patients. Incorporating digital health and ensuring clear standards should be top priorities for India's legal framework revision, stated this report. Currently, people are debating how to enhance India's thriving health-data ecosystem with fresh concepts. In this post, we will look at how India's healthcare and regulatory institutions can be adapted to establish a safety monitoring system that is strong, flexible, and globally networked. This approach serves to protect public health while also positioning India favorably in the global market for medical equipment and medications.



DRA-PM-002

Evaluating the Effectiveness of Detection Technologies in Combating Substandard, Spurious, Falsely Labeled, Falsified and Counterfeit drugs (SSFFC).A Systematic Review

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Objective: The objective of this review is to systematically assess the efficacy of interventions to address the challenges of identifying SSFFC medications.

Method: A systematic search was executed across multiple databases, including pubmed/Medline, EMBASE, Google Scholar and Web of Science and grey literature from 2004 to July 2024. Observational and Analytical studies were included. Systematic reviews, meta-analyses and narrative reviews were excluded that do not present original data. Two reviewers independently completed in duplicate, the study selection and data ions. We registered the protocol in PROSPERO, an international prospective register of systematic reviews (CRD42024598 808).

Results: 26 studies out of 10,444 citations met the criteria for inclusion. Most of them (84.62%) concentrated on analytical methods, with pharmacosurveillance (7.69%) and product development (7.69%), respectively. It contains 22 studies on analytical technology from both developed and developing nations. Two of the studies concentrate on supply chain management in Bangladesh and the United States, while the other two studies examine 2D technology and QR codes in China and Europe. Analytical studies focused on the matter like cost-effectiveness, efficiency, reliability, and the capacity to identify substandard medications. Analytical investigations encountered difficulties with techniques that were only appropriate for crystalline materials, confirmatory test failures caused by overlapping spectra, and restricted applicability to specific drug samples. While product development faced challenges like complicated sample preparation and pharmacosurveillance's difficulty tracking counterfeit medications outside of authorized channels,

Conclusion: The development of interventions to address the problems with SSFFC drugs depends on a number of factors. There is little data on their effectiveness, dependability, and capacity to identify SSFFC medications. In order to lower the prevalence of SSFFC drugs, policymakers and stakeholders must fortify the regulatory framework and implement supply chain technology to improve post-market surveillance, where further research is required.



DRA-PM-003

Navigating Personalized Medicine Global Regulatory Perspectives and Future Directions

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Personalized medicine incorporates environmental, genetic, and lifestyle data to deliver individualized prophylactic and treatment strategies. Although cancer therapeutics has pioneered personalized medicine, its spectrum is expanding into neurology, cardiology, and infectious disease. While, global regulatory framework delay at the back of scientific advancement, was hindered by sophisticated multi component diagnostics, data privacy, AI integration and confined availability in low- and middle-income countries. This study uses comparative regulatory analysis of global agency frameworks to examine convergence, divergence, and challenges in personalized medicine, focusing on timelines, biomarker validation, companion diagnostics, and real-world evidence integration. In the United States, the FDA has led efforts like the Precision Medicine Initiative, Breakthrough Device Designation, and genetic guidance for companion diagnostics. The EU, through the EMA, is adding personalized medicine to its frameworks with adaptive pathways, PRIME, and Horizon Europe initiatives. Japan's PMDA is known for its Sakigake fast-track program. Meanwhile, India is working on improving its regulatory framework, with draft guidelines from CDSCO and help from the Indian Council of Medical Research (ICMR). To fully harness Personalized medicines potential globally, the regulatory system will be synchronized with adaptive trial methods and overseen by an artificial intelligence. National funding will be allocated to federated real-world evidence (RWE) infrastructure and clinical education. New policies should be implemented to ensure cost-effectiveness and encourage digital accessibility.



DRA-PM-004

A Comparative Study of Drug Pricing Regulations in Developing Countries

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Background:

It is consistently difficult for developing countries to guarantee access to reasonably priced, high-quality medications. The extent and enforcement of drug pricing regulations vary and is quite expensive. Such countries depend on WHO Prequalification or from stringent regulatory authorities to ensure the quality and safety of medical products. The lack of visibility of regulatory requirements in developing countries can result in higher costs and patients' delayed access to drugs.

Aims & Objectives:

The aim is to provide recommendations enhance the existing pharmaceutical pricing regulations in developing countries

The objective is to propose strategies for strengthening regulatory frameworks that improve affordability, accessibility and transparency in drug pricing.

Methods:

A qualitative policy analysis was conducted using WHO Global Benchmarking Tool, Health Action International (HAI) pricing surveys and national regulatory data. Pricing models, statutory authority, and enforcement mechanisms in developing countries were assessed. Recommendations were based on WHO pricing guidelines and WHO GBT maturity indicators.

Results:

The analysis reveals the significant variation in pricing regulation frameworks across developing countries, with many exhibiting limited statutory authority and weak enforcement capacity. Countries with more structured pricing models and higher GBT maturity levels demonstrated better affordability and availability of essential medicines. Gaps were identified in policy implementation, transparency and regulatory consistency. Best practices from developed countries systems to be recommended for regulatory strengthening.

Conclusion:

To enhance drug pricing regulations in developing countries, the WHO GBT framework provides a structured roadmap for identifying regulatory gaps, improving transparency and building patient-centered, uniform pricing mechanisms.

Countries with clearer pricing policies and stronger regulatory systems demonstrated better affordability and access to medicines. Strengthening regulatory capacity, improving transparency and adopting context-specific pricing strategies are essential for achieving equitable access to essential medicines.

Keywords: Drug pricing regulation, statutory authority, WHO Global Benchmarking Tool, Health Action International.



DRA-PM-005

Electronic Source Data Compliance: Aligning FDA and EMA Expectations in a Digital World

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Background:

The shift toward digital platforms has positioned electronic source data (esource) as a key asset in modern clinical trials. Esource enables real-time data capture, minimizes transcription errors, and enhances data traceability—improving overall data integrity, transparency, and regulatory confidence. However, its global adoption is challenged by differing regulatory expectations. Notably, the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) offer varying guidance, creating compliance complexities that hinder seamless international implementation.

Aims & Objectives:

This study aims to critically evaluate and compare FDA and EMA regulatory expectations on Electronic Source usage in clinical research. The objective is to propose a harmonized strategy that supports dual compliance and promotes efficient global trial execution.

Methods:

A comparative review of key regulatory documents was conducted, including FDA's Guidance on Electronic Source Data in Clinical Investigations (2013), Title 21 CFR Part 11, and EMA's guidance under eudralex Volume 10 and 11. Core evaluation criteria included system validation, audit trails, data accuracy, access control, and remote monitoring support.

Results:

Both agencies emphasize data integrity, reliability, and security. FDA guidance is more prescriptive, stressing compliance with Part 11 and ALCOA+ principles (Attributable, Legible, Contemporaneous, Original, Accurate, and Complete). EMA promotes a flexible, risk-based approach while upholding Good Clinical Practice (GCP) standards. Common gaps include inadequate audit trail implementation, insufficient system validation, and ineffective access controls.

Conclusion:

Despite linguistic and procedural differences, FDA and EMA share aligned objectives in ensuring credible electronic data. A harmonized approach—including validated systems, strong documentation, and risk-based oversight—can bridge regulatory gaps. Such alignment is critical for enabling compliant, innovative, and efficient digital clinical research across global settings.

Keywords: esource, FDA, EMA, regulatory compliance, electronic records, clinical trials, data integrity



DRA-PM-006

Approach of Digitalizing Prescription for Drug Control and Monitoring the Regulatory Affairs of Drug's Buying Capability Among The People

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The fundamental Approach on the “Digitalization of Prescription” is to enrich the capability of the Individual Prescription role and its value of correspondence, and responsibilities among the public by (Systemised Approach on Regulating Prescription and Randomized Interface Youngish Application). Is a techno-based module of customizing the prescription in a randomized digital version with a Unique Identifying Number (UIN) and validating the prescription in every Drug Store. “Digitalizing Prescription” is the concept of Unleashing the practicing of buying Drug's from the Medical Store according to the Prescription and the Pros & Cons of the prescription handling in society and ill effect of unaccountable prescription practicing. Discussing the Fundamentals of Digitalizing the prescription to avoid the unnecessary drug is available for Registered Doctors and Pharmacists on verifying and controlling the Drug Distribution to the patient on Recommended level by authorizing the prescription by the UIN (Unique Identifying Number) Generated by the Application on Randomized Manner. By using the Randomized number able to Monitor the prescription and to control the level of Narcotics and Non-OTC (Over the Counter) drug's supply chain management, the motive of the Research is to Characterizing the Prescription and discussing the outcome of Research into a detailed conversation, and the Solution to the Problems faced by Drug's Distribution among the society and the Unaccountable Prescription, which on changing the unaccountable to the accountability.

Keywords: Digitalizing Prescription, UIN (Unique Identifying Number), Artificial Intelligence (AI).



DRA-PM-007

Accelerated Approval Mechanism: Fast-Tracking the patient access to life saving research

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Background:

The Accelerated Approval Mechanism (AAM) is a regulatory pathway introduced by the U.S. Food and Drug Administration (FDA) in 1992 to expedite the approval of drugs that treat serious or life-threatening conditions, especially where there is an unmet medical need. This mechanism allows drug approvals based on surrogate endpoints that are reasonably likely to predict clinical benefit, rather than waiting for direct evidence of long-term therapeutic outcomes.

Aim: Study of accelerated approval mechanism for emergency approval of medicines.

Objectives: To evaluate the accelerated approval pathway as a regulatory tool that bridges pharmaceutical research with urgent, unmet therapeutic needs

Methods:

A comprehensive literature review of regulatory guidelines (FDA, EMA), journal articles, and real-world case studies has been performed. A comparative evaluation has been undertaken on the drugs approved via the AAM from 2010–2024, focusing on therapeutic areas, endpoints used and post-marketing commitments.

Results:

The accelerated approval mechanism significantly reduced time-to-market for novel therapies in oncology and vaccines or medicines for infectious diseases. In oncology, **Pembrolizumab (Keytruda)** received approval for multiple cancers (e.g., non-small cell lung cancer, melanoma) based on surrogate endpoints like **tumor response rates** and **progression-free survival**. In infectious disease, **Remdesivir** received accelerated approval during the COVID-19 pandemic, based on endpoints such as **reduced viral load and shortened recovery time**. Thus, the surrogate endpoints such as tumor shrinkage and viral load played a critical role. However, approximately 30% of drugs required additional post-marketing studies to confirm long-term benefits, leading to regulatory reassessment in some cases.

Conclusion:

The accelerated approval pathway exemplifies how regulatory innovation can align with scientific advancement to enhance patient access. While offering hope for high-risk patients, it also underscores the need for robust post-approval surveillance and ethical oversight to maintain public trust and therapeutic value.

Keywords:

Accelerated approval, FDA, Surrogate endpoints, Fast-Tracking, Therapeutic outcomes, Post-Marketing studies



DRA-PM-008

Comparative analysis of USA, EU and India with recommendations for strengthening, India's veterinary medicine regulation.

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Veterinary medicine plays important role in enhancing the safety efficacy and well being of animals and also implication on human health. Approval pathways and post marketing approval of veterinary medicines regulations is different in United states (US) European union (EU) and India. In USA centre for veterinary medicine (CVM), is responsible for monitoring animal drug, feed, medical devices and also provides guidance for industry, consumers and veterinarians. In European union is responsible for monitoring research and development and marketing authorization and post marketing authorization of veterinary medicinal products. In India the Central drug control standard organization (CDSCO) is the key regulatory body which performs vital functions in approval of drugs and biologics, testing, licencing and post marketing approval of veterinary medicines. Despite there is a certain challenge includes lack of standardized regulations and guidelines, deficiencies in pharmacovigilance, limited digital infrastructure, ethical and animal welfare oversight, bioequivalence protocol variability. In India veterinary medicines lacks of dedicated specific guidelines less regulatory focus lack of guidelines on veterinary clinical trials, lack of pharmacovigilance program and post marketing surveillance is limited. In ordered to combat these gaps, India should adopt a separate regulatory division within CDSCO; to enhance clinical trials oversight by standardization and digitalization this streamlines the approval pathways and strengthens the post marketing surveillance.



DRA-PM-009

Regulations in Special Populations & Special Scenarios Pediatric Drug Development

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Background:

In order to guarantee safe and efficient treatments for kids, pediatric drug development poses particular regulatory opportunities and challenges that call for specialized regulatory frameworks. To encourage and require pediatric studies concurrent with adult drug development, regulatory bodies around the world, such as the FDA, EMA, PMDA, and others, have created specific legislative acts and guidance.

Aims:

Establish regulatory frameworks that guarantee pediatric populations receive therapies that are rigorously evaluated for safety, efficacy, and quality to encourage the submission of pediatric development plans early in the drug development process.

Objectives:

To mandate and facilitate studies on children (pediatric populations), close Pediatric Access Gaps and Encourage Collaboration

Methods:

Pediatric Research Equity Act (PREA) and Best Pharmaceuticals for Children Act (BPCA) require and incentivize pediatric studies, respectively. Pediatric Investigation Plans (pips) are mandated early in development and must be approved by the Pediatric Committee (PDCO) Submission of an initial Pediatric Study Plan (ipsp) is required for new drug applications, detailing proposed pediatric studies, age groups, formulations, and timelines.

Results:

In Overall, collectively guides regulatory agencies and stakeholders in advancing pediatric drug development, ensuring that children benefit from timely, safe, and effective therapies tailored to their unique needs with ethical protections. They also encourage cooperation between the industry, regulators, and patient groups to improve treatment outcomes for kids around the world.

Conclusion:

This regulatory framework helps make sure that pediatric medicines are available on time by evaluating strict scientific review with regulatory body and ethical precautions. It make sure pediatric drug development initiatives as good as they can potentially be better health outcomes for children throughout the global.

Keywords: Pediatric drug development, Regulatory frameworks, FDA, EMA, PMDA Pediatric Research Equity Act (PREA), Best Pharmaceuticals for Children Act (BPCA), Global harmonization, Pediatric Investigation Plans (pips), Ethical considerations, Specialized medicines, Special populations.



DRA-PM-010

Tackling regulatory and ethical challenges in personalised medicines

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Background: Personalised medicine aims to customise medical treatment based on an individual's genetic makeup, lifestyle, and environment ^[1]. This approach promises to improve therapeutic outcomes, minimise adverse reactions and optimise healthcare resources. Shift towards personalised medicines brings with it challenges to regulatory compliance as well as commercial manufacturing. The very nature of dosage forms is responsible for this. Various regulations, qtps and cqs of conventional drug delivery systems have been reviewed to arrive at certain conclusions.

Aims & Objectives: The aim is to identify, analyze and propose the strategies to overcome regulatory and ethical challenges in Personalized medicines.

Objectives

- To identify gaps in current regulatory frameworks for approving targeted therapies and companion diagnostics
- To analyze ethical concerns regarding patient consent, data privacy, and equitable access
- To propose practical strategies to address these barriers and facilitate innovation translation

Methods: A review of key regulatory guidelines like ICH E6(R3) GCP draft, EMA Guideline on Good Pharmacogenomic Practice, FDA Guidance for Industry on In Vitro Companion Diagnostic Devices and policy frameworks like General Data Protection Regulation have been performed. Recent examples of adaptive trial designs and Real-World Data (RWD) applications are also reviewed to assess feasibility and compliance considerations.

Results: Findings indicate that fragmented global regulatory standards, complex co-approval processes for companion diagnostics, and limited integration of Real-World Evidence (RWE) hinder timely approvals of Personalized medicines. Ethical challenges persist around genomic data protection, and potential complications for an efficient implementation at patient level. Solutions include harmonizing global guidance, strengthening data governance, adopting adaptive pathways, careful selection of dosage forms, education of healthcare professionals and enhancing patient engagement.

Conclusion: Successfully advancing personalized medicines demands addressing fragmented regulatory frameworks and complex ethical considerations through global harmonization, stronger data governance, and adaptive regulatory pathways. Implementing clear co-approval processes for companion diagnostics, safeguarding genomic data privacy, and enhancing stakeholder awareness can significantly improve patient access and trust. These strategies collectively facilitate the safe, efficient, and equitable translation of personalized medicine innovations from research to real-world clinical practice.

Keywords:

Personalised medicine, regulatory science, ethics, companion diagnostics, adaptive trials, genomic data, real-world evidence.



DRA-PM-011

Global Medical Device Adverse Event Coding - FDA

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Background: Advances in insulin delivery, particularly through insulin pump therapy, continue to transform diabetes management by improving glycaemic control. However, these technologies also introduce new safety risks. This article examines global medical device adverse event coding through two case reports involving Medtronic Mini Med 530G and Mini Med 670G insulin pumps.

Objectives: To emphasize the need for stronger device surveillance and patient safeguards.

Methods: Case 1 involves a patient with type 2 diabetes who experiences severe hypoglycaemia due to a motor malfunction in the pump, resulting in uncontrolled insulin release and requiring intensive care. Case 2, sourced from the FDA's MAUDE database, highlights severe hypoglycaemia with seizures following a pump crack and CGM (Continuous Glucose Monitor) failure.

Results: Both cases are categorized under the International Medical Device Regulators Forum (IMDRF) coding framework, revealing mechanical and electrical failures, inadequate safety interlocks, and weak design integrity. Common device vulnerabilities include unreliable motor mechanisms, fragile structural components, and ineffective CGM integration.

Conclusion: The analysis highlights critical needs for improved device engineering, mandatory CGM redundancy, and robust post-market surveillance. Collaborative efforts among manufacturers, healthcare providers, and regulators are essential to strengthen design standards and enhance patient safety.

Keywords: CGM, FDA, IMDRF, Insulin Pump, MAUDE, PMS



DRA-PM-012

The Effect of The European Artificial Intelligence Act on Medical Devices

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Background: The integration of artificial intelligence (AI) into medical devices is reshaping the healthcare sector, offering both transformative opportunities and complex regulatory hurdles.

Objectives: To address challenges introduced the Artificial Intelligence Act (AI Act) a pioneering legal framework designed to govern AI applications in EU.

Methods: The AI Act on AI-driven medical technologies, particularly within the context of the Medical Device Regulation (MDR) and In Vitro Diagnostic Regulation (IVDR). Given that AI-powered medical tools are predominantly classified as high-risk, manufacturers are obligated to meet rigorous criteria involving data integrity, risk management, transparency, and human supervision.

Results: Study explores the overlapping regulatory domains between MDR/IVDR and the AI Act, including post-market monitoring and documentation standards. Special attention is paid to adaptive AI systems, which evolve post-deployment and present unique regulatory considerations.

Conclusion: The global ripple effects of the Act popularly known as the "Brussels Effect" are also analyzed, demonstrating its extraterritorial influence on non-EU developers. Overall, the AI Act marks a critical advancement in fostering safe, ethical, and innovative use of AI in the medical field.

Keywords: European Union (EU), Medical device regulations (MDR), Medical Device, Artificial Intelligence Act (AIA).



DRA-PM-013

Exploring the Challenges Faced by Generic Version of Complex Drugs: A Scoping Review

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Background: Complex generic medicine has transformed the global perception of generic medicaments. Complex generics include complex active pharmaceutical ingredients (apis), formulations, dosage forms, routes of administration and drug device combinations.

Aim & Objective: The present review aims to investigate the challenges faced by different stakeholders and the strategies adopted to address these challenges during the development and approval stages of complex generics.

Method: We followed the Preferred Reporting Items for the Scoping Reviews Extension for Systematic Reviews and Meta-Analyses (PRISMA-scr) guidelines. One thousand seven hundred eighteen publications were found after searches of pubmed, EMBASE, Scopus, and Web of Science from January 1, 2014, to August 22, 2024. Two authors independently reviewed the retrieved papers to reduce the possibility of bias. After the titles and s of the articles were examined, the texts were screened according to predetermined inclusion and exclusion criteria. The facts and conclusions of the investigations were also examined regarding challenges and strategies.

Results: A total of 1718 studies were retrieved from the database searches, from which twenty-four of the obtained articles were included. The formulation challenges (17 articles), analytical challenges (19 articles), clinical challenges (18 articles), critical process parameter-related challenges (17 articles), critical quality attribute-related challenges (19 articles), and regulatory challenges (21 articles) were the major challenges of complex generics.

Conclusion: The use of advanced sophisticated analytical equipment as well as orthogonal bioanalytical testing, the implementation of a dynamic regulatory cross-checking system, the development and use of machine learning and artificial intelligence tools, the development of quality-by-design approaches and models have been recognized as the best methods for addressing these challenges and present great opportunities in terms of complex generics growth.



DRA-PM-014

Navigating Global Regulatory Challenges in the Era of Post Pandemic Pharmaceutical Supply

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Background: The global pharmaceutical industry is facing increasingly complex regulatory challenges, especially after the COVID-19 pandemic. With rapid advances in technology and the growing demands of globalized markets, there's now a stronger need for consistent regulations that ensure both patient safety and smooth market access.

Aims & Objectives: This review looks at how the pandemic affected pharmaceutical regulations and supply chains around the world. It also explores the adjustments and innovations that have helped the industry become more resilient and compliant in this evolving landscape.

Methods: An in-depth literature review was conducted, focusing on the regulatory responses from key regions such as the United States, European Union, and China. The study also examined the role of digital technologies and international collaboration in overcoming regulatory and supply chain challenges during and after the pandemic.

Results: COVID-19 revealed major weaknesses in existing regulatory systems and supply chains, prompting faster and more flexible approaches to drug approval and monitoring. Each region adapted differently—while the U.S. emphasized speed, the EU prioritized inclusivity, and China focused on modernization. The adoption of tools like artificial intelligence, blockchain, and remote inspections has significantly improved compliance and real-time monitoring. Cross-border cooperation also became more prominent, leading to quicker approvals and better post-market safety tracking.

Conclusion: The pandemic has driven lasting changes in pharmaceutical regulation. With increased use of technology, improved flexibility, and stronger global cooperation, the industry is now better prepared to face future public health emergencies.

Keywords: Pharmaceutical regulation, Post-pandemic resilience, Supply chain management, Regulatory innovation, Digital health technologies



DRA-PM-015

From Paper to Predictive: The Evolution of Regulatory Submissions with AI.

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Background: Traditional regulatory submission processes, with their stringent compliance measures and complex documentation, have taken a back seat due to their inability to keep up with increasingly complex and time-sensitive demands in the health and pharmaceutical sectors.

Aims and Objectives: This study focuses on exploring how AI enhances regulatory submissions and compliance, while identifying associated challenges and ethical considerations, particularly in Machine Learning and Natural Language Processing (NLP).

Methods: The review covered AI applications in streamlining dossier creation, optimizing change control, and enhancing audit readiness. Relevant studies were analysed thematically to identify improvements in efficiency, compliance, risk prediction, as well as challenges related to data ethics and regulatory harmonization.

Results: There are measurable improvements which are demonstrated by AI-enabled platforms such as reduced submission times, enhanced data integrity, and smarter risk prediction models. NLP automates document summarization and regulatory text analysis, while machine learning real-time compliance tracking. However, issues around data ethics, transparency, and regulatory harmonization present ongoing challenges.

Conclusion: AI is no longer just a future prospect; it represents a transition from paper-based processes to predictive, intelligent automation, making it an operational imperative. By embracing AI technologies such as machine learning and NLP for regulatory text analysis and real-time compliance tracking, industries can improve efficiency. However, challenges around data ethics, transparency, and regulatory harmonization remain significant.

Key Words: Artificial Intelligence, Audit readiness, Compliance Automation, NLP, Regulatory submissions.



DRA-PM-016

One Product, Two Rules: The Global Struggle of Regulating Drug-Device Combinations.

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Background:

Drug Device combination products are transforming the modern healthcare with integrated systems offering precision, innovation and convenience. While these leading-edge technologies elevate the standard of care, they also have significant flaws in global regulatory frameworks. The combination of drugs and devices creates a grey area where manufacturers and regulators face issues in classification, overlapping jurisdictions which results in delay of marketing approval.

Aims & Objectives:

To identify the regulatory roadblocks in the approval of Drug-Device Combination Products across USA, EU, Japan, Malaysia, and Nigeria and to propose actionable strategies for accelerating efficient global market access.

Methods:

This study employed a qualitative analysis of regulatory frameworks for the approval of Drug-Device combination products. The data were collected from official regulatory agency documents and peer-reviewed literature to analyze challenges in approval frameworks across five countries. Key challenges from these resources were identified and strategies to harmonize global regulatory approaches were proposed.

Results and Conclusion:

Despite varying stages of regulatory maturity, all five regions face difficulties in defining, evaluating and approving combination products. Like in USA, the main challenge is the classification criteria whereas in Europe it is insufficient regulatory guidance. Harmonized guidance, inter-agency coordination, and investment in regulatory infrastructure are crucial to streamline global approvals and ensure patient access to innovative therapies.

Keywords:

Approval Changes, Combination Products, Drug-Device Combination Products, Harmonization, Regulatory Framework.

DRA-PM-017

Current Status of Maternal Health in India: A Regulatory Overview

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Maternal health is still a cause of public health concern in India, especially with regard to ongoing inequalities in access to quality services among rural and underserved populations. Anaemia, hypertensive disorders, haemorrhage, and sepsis are the main causes of maternal morbidity and mortality. Even though national programs like RMNCH+A and activities under the National Health Mission have enhanced service delivery, the regulatory environment for maternal health interventions remains weak.

The Central Drugs Standard Control Organization (CDSCO) regulates drugs and devices but does not have focused policies for pregnancy products. Pregnant women are not given access to clinical trials on a routine basis due to ethical limitations, leading to inavailability of population-specific safety and efficacy information. There is no regulatory advice on approving combination products (such as drug-device therapies) employed in obstetric practice, and pharmacovigilance systems do not effectively track adverse effects in pregnancy.

In comparison, international regulators like the US FDA and EMA have implemented structured systems of pregnancy labelling and risk assessment guidelines. India needs to implement similar strategies, such as maternal pharmacovigilance specifically designated, ethical research inclusion, and regulatory pathways tailored to pregnancy. Increasing regulatory oversight is crucial to safe, evidence-based maternal care as well as the accomplishment of Sustainable Development Goal 3.1 to decrease preventable maternal deaths globally by 2030.



DRA-PM-018

FDA's Risk-Based Approach to Control of Nitrosamine Impurities in Pharmaceuticals

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Carcinogenic nitrosamines have raised considerable safety concerns regarding pharmaceutical product safety due to their impurity status. In line with this, FDA has developed a risk-based comprehensive framework for its control. The FDA guidance adopts an approach guided by risk assessment through a tiered mitigation strategy that requires manufacturers to: analyze the risks of APIs and drug products thoroughly; carry out confirmatory testing, where risks are identified; and report any changes to comply with regulatory requirements that reduce or prevent nitrosamine levels. The fundamental changes made in the recent guideline included differentiating between common nitrosamines and ndsris (nitrosamine drug substance-related impurities), as well as imposing revised acceptable intake limits based on assessments of carcinogenic potential. ICH Q2(R1) validation of methods is required, with appropriate sensitivity and specificity against the regulatory threshold. The FDA stresses proactive risk assessment, analytical vigilance, and continual process optimization including the stringent control of raw materials excipients and packaging. This guidance allows flexibility that permits the use of scientifically justified alternative approaches for instances of multiple nitrosamines all with the goal of ensuring that total nitrosamine exposure does not exceed a lifetime cancer risk of 1:100,000 as defined by ICH M7(R2). These measures reflect the FDA's rigorous impurity monitoring and control exhibiting the agency's commitment to public health in harmony with expectations of global regulators.



DRA-PM-019

Real Time Pharmacovigilance-An Overview

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Background:

Pharmacovigilance (PV) is crucial in ensuring drug safety, yet traditional systems often face issues like delayed signal detection and underreporting. With healthcare data becoming increasingly digital, there is an urgent need for real-time solutions that can identify adverse drug reactions (adrs) more efficiently. Real-time pharmacovigilance (RTPV) integrates digital tools, data analytics, and artificial intelligence to proactively monitor drug safety.

Aims & Objectives:

This review aims to provide a comprehensive overview of real-time pharmacovigilance, including its data sources, implementation strategies, global regulatory perspectives, benefits, limitations, and future directions. The objective is to highlight RTPV's potential in enhancing patient safety and regulatory responsiveness through continuous and automated surveillance.

Methods:

A structured literature review was conducted using scientific databases, regulatory guidelines, and real-world program documentation. Key themes explored include data acquisition from electronic health records (ehrs), mobile apps, social media, wearables, and integration of AI/ML models for signal detection. Real-world applications like FDA Sentinel, EMA eudravigilance, and pvpi were critically analyzed.

Results:

Findings indicate that RTPV enables faster ADR signal detection, improved clinical outcomes, and better regulatory compliance. It utilizes big data, predictive modeling, and real-time dashboards for continuous risk management. Despite challenges in data privacy, standardization, and algorithm bias, RTPV offers transformative potential in pharmacovigilance.

Conclusion:



Real-time pharmacovigilance represents the next evolution in drug safety. Its integration into regulatory frameworks and healthcare systems worldwide can significantly enhance pharmacovigilance efficiency, enabling proactive responses to drug-related risks and improving public health outcomes.

Keywords: Adverse Drug Reactions (adrs), Drug Safety Monitoring, Electronic Health Records (ehrs), Signal Detection, Mobile Health.



DRA-PM-020

IVDR Watch: European Regulators Update Implementation Framework.

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Background: The In Vitro Diagnostic Regulation (IVDR) (EU 2017/746) represents a significant shift in the regulatory landscape for in vitro diagnostic medical devices in the European Union. The IVDR, which took the place of the preceding IVDD (98/79/EC). A more comprehensive framework for performance evaluation and post-market surveillance is provided, along with robust conformity assessment procedures and a risk-based classification system.

Aim: To increase market transparency, strengthen regulatory oversight, and enhance patient safety for medical devices in the EU.

Objective: To represents a significant shift in the regulatory landscape for in vitro diagnostic medical devices in EU.

Methods: All ivds bearing the CE mark are required to undergo new evaluations, unless they are excluded from specific transitional terms, such as the "Grace Period" or the "Sell-off Provision." This is one of the primary characteristics of the regulation. The guideline calls for comprehensive technical documentation, UDI (Unique Device Identification), and registration in the EUDAMED database in order to increase traceability.

Results: The responsibilities of EU Reference Laboratories, Notified Bodies, and Expert Panels have been expanded, especially for high-risk (Class D) devices. Manufacturers must follow stringent General Safety and Performance Requirements (gsprs) and have up-to-date regulatory documents.

Conclusion: The IVDR improves harmonisation and accountability throughout the EU, but it also poses significant compliance challenges, particularly for smaller companies. Nonetheless, the regulation promotes innovation and increases the safety and transparency of the European diagnostics market.

Keywords: In Vitro Diagnostic Medical Devices, European Union In Vitro Regulation, EU Declaration of Conformity Process, CE Marking for Medical Devices, General Safety and Performance Requirements.



DRA-PM-021

Nutraceuticals At the Crossroads: Ip Challenges, Clinical Research & Its Strategic Opportunities

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Background:

The global nutraceutical industry is rapidly expanding, driven by increased consumer awareness of health and wellness. However, the industry faces challenges related to product safety, regulatory disparities, and intellectual property protection. Adulteration, mislabeling, and lack of clinical validation often hinder public trust and effective market growth.

Aims & Objectives:

This review aims to examine the intersection of intellectual property rights (IPR), clinical research, and regulatory practices in the nutraceutical industry. It also seeks to identify challenges, opportunities, and future strategies to enhance product safety, innovation, and accessibility.

Methods:

A comprehensive literature review was conducted using databases such as pubmed, Elsevier, Cambridge, Springer, and online platforms. The study evaluated regulatory guidelines, case studies, global market trends, clinical trials, and patent filings from 2016 to 2024 using targeted keywords like "Nutraceuticals," "IPR," "Clinical Trial Regulations," and "Public Health."

Results:

Findings revealed significant gaps in harmonized regulatory frameworks, ethical marketing practices, and quality control mechanisms across different regions. Only 45% of consumers could define nutraceuticals correctly, and 30% expressed doubts regarding their efficacy. Clinical trials remain underfunded, and many products lack scientific backing. However, innovative strategies such as AI-driven R\&D, GMP adherence, and international collaborations are being adopted. Companies investing in clinical research and IP protection have reported a 20–25% increase in market share.

Conclusion:

A sustainable nutraceutical industry requires balanced integration of intellectual property protection, regulatory compliance, and ethical marketing. Collaborative efforts between governments, industries, and academia are essential to ensure product integrity, foster innovation, and protect public health. The future lies in harmonized standards, consumer education, and leveraging emerging technologies for clinical and regulatory advancements.

Keywords:

Nutraceuticals, Intellectual Property Rights (IPR), Clinical Trials, Public Health, GMP, Adulteration, Regulation, Innovation, Consumer Safety



DRA-PM-022

A Revolutionary Digital Architecture for Boosting Biomedical Research Systems' Data Integrity

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As digital data grows rapidly, biomedical research needs data management that is transparent, secure, and immutable. Clinical research data and findings face threats from unauthorized access, manipulation, and potential loss. This paper suggests a digital platform based on distributed ledger technology to enhance the security, transparency, and reliability of biological research records. Decentralized, cryptographically secure data structures enable unchangeable record-keeping, real-time access control, and verifiable audit trails across investigations involving multiple institutions. Modern informatics shows how digital systems can enhance data sharing, reduce fraud, and ensure compliance with regulations while maintaining anonymity. Numerous regulatory, ethical, and practical challenges need to be overcome to implement good clinical practice (GCP). The paper concludes by discussing smart contracts, technology mergers, and the necessity of global standards for seamless integration. This innovative strategy has the potential to enhance patient care and strengthen the credibility of scientific findings by reinforcing clinical research ecosystems, making them more reliable, transparent, and effective. Implementing GCP brings about various operational, ethical, and regulatory challenges. The article wraps up by addressing smart contracts, the merging of technologies, and the need for global standards to enable seamless integration. This new approach has the potential to strengthen clinical research ecosystems, making them more robust, transparent, and reliable, ultimately improving patient care and scientific legitimacy.



DRA-PM-023

Cardiac Medical Device Regulations in the USA, EU & Japan: A Comparative Study

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Cardiac medical devices are essential for diagnosing and treating cardiovascular diseases, the leading cause of death globally. As innovation accelerates and technologies like AI/ML become integral to device development, regulatory frameworks must adapt to ensure patient safety, timely access, and market readiness. This study presents a comparative analysis of cardiac medical device regulations across three major regions-the United States, European Union, and Japan. Using a structured methodology grounded in IMDRF principles, it examines classification systems, pre-market approval pathways, post-market surveillance, and the integration of advanced technologies. Key findings reveal significant variations in regulatory costs, approval timelines, enforcement intensity, and harmonization with international standards. While all three regions employ risk-based classification and emphasize clinical evidence, unique challenges persist, such as navigating the EU's MDR, Japan's language and harmonization barriers, and the U.S.'s balance between innovation and safety. The study highlights the importance of global regulatory convergence to streamline processes, foster innovation, and enhance patient outcomes in cardiac care.



DRA-PM-24

Regulatory and Toxicological Considerations of 3D-Printed Microneedles: A Systematic Review of Global Compliance and Standardization Challenges

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3D-Printed Microneedles (MN's) are most innovative minimally invasive drug delivery and diagnostic tool or a device which are subclass of Transdermal Drug Delivery Systems. 3D-Printing technology allows microneedles to be personalized or customized and allows rapid prototyping. While there is an exponential growth in technologies, regulatory frameworks and toxicological assessment methods still needs adaptation. This systematic review evaluates current regulatory approach, toxicological considerations, and challenges in standardization with respect to 3D printed mns. A defined research statement will be established based on the Population Intervention Comparison and Outcome usually referred as PICO framework. A comprehensive literature review will be conducted in adhering to PRISMA 2020 guidelines. Relevant peer-reviewed articles and regulatory documents will be collected using defined search strings and keywords across various databases. This analysis emphasizes the regulatory readiness across various regulatory bodies like., United States Food and Drug Administration (USFDA) evaluates 3D-Printed mns on case-by-case basis, requiring various data on biocompatibility, validation of process and reproducibility, but lacks device specific guidelines similarly the regulatory frameworks across the world for 3D-Printed Microneedles are deficient and are usually regulated by various coincided regulations. This review highlights the need of cohesive, device-specific regulatory pathways and harmonized toxicological standards to ensure the safety and effectiveness of 3D-Printed microneedles in biomedical healthcare applications.



DRA-PM-025

Challenges to the ivds Manufacturers in the WHO Pre-qualification Assessment

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Background:

The World Health Organization (WHO) Prequalification Programme plays a pivotal role in ensuring the quality safety and performance of in vitro diagnostic (IVD) products particularly in resource-limited settings. The process begins with determining a products eligibility for assessment followed by a pre-submission phase where manufacturers submit a request via the epqs portal. Upon review WHO may invite the manufacturer for either a full or abridged prequalification assessment.

A full assessment includes a comprehensive review of the product dossier, performance evaluation manufacturing site inspection and labelling review. In cases where a product has already received regulatory approval from a stringent authority WHO may consider an abridged assessment which aims to reduce redundancy while focusing on aspects critical to global public health impact.

Aims & Objectives:

To evaluate the regulatory and technical challenges encountered by IVD manufacturers during the WHO prequalification assessment process.

Methods:

Literature Review Initiation: Conduct a systematic literature review using databases such as pubmed, Scopus, Google Scholar, WHO Prequalification (pqdx) frameworks.

Results:

The study identified key challenges such as regulatory complexity, dossier preparation, and high compliance costs. These barriers highlight the need for clearer guidance and stronger support to improve global access to quality diagnostics.

Conclusion:

The World Health Organization (WHO) Prequalification Programme ensures the quality safety and performance of in vitro diagnostic (IVD) products particularly for use in resource limited settings. The process begins with determining a products eligibility followed by a pre-submission and either a full or abridged assessment. During this programme, which enhances global health access, ivds manufacturers face several challenges during the assessment. These include regulatory complexity navigating evolving WHO and IMDRF guidelines and. Performance evaluations in simulated low -resource settings labelling and language compliances and high financial burdens further complicate the process. Moreover, post qualification commitments such as annual reporting surveillance and change management require sustained regulatory oversight. Addressing these challenges is crucial to enabling broader participation in WHO prequalification programme and improving the availability of quality-assured diagnostics globally.

Keywords:

WHO Prequalification, In Vitro Diagnostics (IVDs), Prequalification Assessment.

DRA-PM-026

Navigating the Regulatory challenges of new age technology based medical devices: A Global Scoping Review

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Objective: The integration of new technologies such as artificial intelligence (AI), machine learning (ML), 3D printing, and the Internet of Medical Things (iomt) into medical devices is revolutionizing healthcare. Although these technologies have moved ahead faster than the development of regulatory frameworks, leaving a vast gap to be filled, there are universal concerns that exist. This scoping review was aimed at comprehensively outlining and categorizing global regulatory challenges concerning such technologies.

Method: This scoping review was carried out as per the PRISMA-scr guidelines. A systematic literature search was performed on four electronic databases, namely Scopus, pubmed, Embase, and Web of Science, from 2014 to 2024. A total of 3,241 records were imported in Rayyan software for effective screening and management. After the removal of 1,368 duplicates, two reviewers in duplicate and independently screened the titles, s, and full texts. Disagreements were resolved by consensus. Of 23 full-text articles that were screened, 8 met the inclusion criteria. Of these, 6 were review or conceptual papers and 2 original research. Articles were also categorized based on technology type: AI/ML (n = 3), 3D printing (n = 3), and iomt (n = 2), with some cross-cutting categories.

Results: The articles included here listed a number of regulatory challenges across technologies. For AI/ML, these were aging approval infrastructures, explainability and undefined accountability. Iomt devices lacked gaps in cybersecurity controls, risk classification, and secure-by-design practices. 3D printing had issues of material inconsistency, post-processing complexity, and documentation needs. Training gaps in. Between practitioners and undefined point-of-care responsibilities, and scattered global regulations, added further to the compliance challenges.

Conclusion: New technology based medical devices promise much but present intricate regulatory challenges beyond safety concern to include cybersecurity, transparency and implementation feasibility. There is a strong need for international harmonized regulatory regimes that can keep pace with new technologies, real-world performance observation and safe inclusion of innovation in healthcare.



DRA-PM-027

Need of Reforming India's Medical Device Regulation: Bridging Gaps and Aligning with Global Standards.

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Background: Medical devices are an integral part of providing good quality of care and healthcare systems, but have been under-regulated in India both in terms of quality and price in comparison to western standards. The explosive growth of this industry, projected at USD 50 billion by 2030, requires a regulatory environment that promotes safety, innovation, and access. The implementation of the Medical Device Rules (2017) has been a step forward, but there remain challenges in enforcement, harmonization, and post-market surveillance.

Aims & Objectives: This paper reviews, analyses and provides critical evaluation on the existing Indian medical devices regulatory ecosystem and suggests the essential structure and programme implementation shortcomings, compares it with global regulatory. More models from European Union, USA and WHO and provides strategic policy recommendations in support of innovation and public health.

Methodology: A structured literature review using regulatory reports, peer-reviewed articles, and policy documents was conducted between 2017 and 2024. The WHO Global Model Regulatory Framework was used as a reference so as to analyse global regulatory frameworks. International standards served as the benchmark for India's system. Comparative analysis was employed.

Result: Findings reveal that while India has adopted a risk-based classification system and digital licensing mechanisms, it lacks adequate infrastructure, trained regulatory personnel, and comprehensive post-market monitoring. In contrast, mature frameworks like EU MDR and US FDA employ robust clinical evaluation, traceability tools, and stakeholder engagement mechanisms. India's dependence on imports and inconsistent enforcement across states further undermine regulatory effectiveness.

Conclusion : India must strengthen regulatory capacity to integrate a unified digital oversight system aligned with global standards. Controls that are stricter after marketing must also be implemented in order to foster innovation that is indigenous. Harmonizing well with international frameworks will not just improve safety but then also make India much more competitive within the global medtech arena.

Keywords: India, of medical devices, regulation, for policy reform, CDSCO, under IMDR 2017, including post-market surveillance, EU MDR, also innovation.



DRA-PM-028

Regulatory Intelligence in Nanomedicines: Bridging Gaps Across the US, EU, and India

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Background

Nanomedicines hold a transformative potential in drug delivery, allowing improved bioavailability, targeted action, and reduced toxicity. Although, their typical physicochemical properties challenge conventional regulatory pathways. Regulatory bodies such as USFDA, EMA, and CDSCO have developed independent guidance and definitions for nanomedicines, leading to divergent requirement in product classification, characterization, safety evaluation and approval processes. These regional variability causes regulatory uncertainty, delayed market access and increased compliance for manufacturers.

Aims & Objectives:

This study aims to assess how Regulatory Intelligence (RI) can mitigate the regulatory fragmentation facing nanomedicines. The specific objectives are:

- To compare nanomedicine related regulatory frameworks across the US, EU and India.
- To identify key regulatory challenges in nanomedicine development and approval.
- To evaluate the role of RI in improving regulatory alignment, submission efficiency and compliance strategies.

Methods:

A qualitative and comparative analysis was performed using official guidance documents from USFDA, EMA and CDSCO, along with peer reviewed literature. A thematic framework was used to categorize definitions, data expectations and approval mechanisms. The role of RI was analyzed by mapping tools, processes, and case examples reported in regulatory science literature

Results:

The findings show significant geographical differences in how nanomedicines are defined, assessed, and approved. India's framework for regulating nanomedicine is still in its infancy, whereas the US and EU have more advanced systems. Common deficiencies include a lack of specified nomenclature, irregular characterization processes, and a lack of post-market surveillance. RI was found to be underutilized, particularly in emerging regulatory regimes, despite its potential to facilitate proactive submission.

Conclusion:

Global patient access can be enhanced, delays can be decreased, and regulatory harmonization can be promoted by incorporating regulatory intelligence into nanomedicine approval processes. It is highly advised that RI be widely adopted, particularly in regulatory contexts pertaining to low- and middle-income individuals.

Keywords: Nanomedicines, Regulatory Intelligence, USFDA, EMA, CDSCO, Harmonization, Regulatory Affairs



DRA-PM-029

Global Perspectives on Fast Track Drug Approvals: Regulatory Frameworks and Challenges

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Background:

The increasing global demand for rapid access to innovative therapies has led to the evolution of fast-track drug approval processes. These expedited pathways are critical for addressing serious or life-threatening conditions where existing treatments are inadequate. However, maintaining a balance between accelerated drug development and ensuring safety and efficacy remains a regulatory challenge.

Aims & Objectives:

This review aims to provide a comprehensive analysis of the fast-track approval frameworks in various countries, including the United States, Europe, Japan, and Australia. The primary objective is to compare standard regulatory pathways with fast-track mechanisms, highlight their unique features, and evaluate their implications on public health and pharmaceutical innovation.

Methods:

A thorough literature review was conducted focusing on the guidelines and policies of global regulatory authorities such as the FDA (USA), EMA (Europe), PMDA (Japan), and TGA (Australia). The study critically assessed expedited programs like Fast Track Designation, Breakthrough Therapy, Accelerated Approval, Priority Review (USA), PRIME (Europe), Sakigake (Japan), and Priority Review (Australia). Key differences in eligibility criteria, review timelines, and post-marketing obligations were compared.

Results:

Expedited approval programs have significantly improved patient access to critical therapies, especially in oncology, antiviral treatments, and rare diseases. However, challenges include reliance on surrogate endpoints, risk of incomplete safety data, and potential post-marketing withdrawals. Case studies such as Imatinib and Remdesivir demonstrate the success of fast-track pathways, while drugs like Ponatinib and Cangrelor highlight associated risks.

Conclusion:

Fast-track regulatory frameworks play a vital role in accelerating drug development for unmet medical needs. However, regulatory agencies must ensure stringent post-marketing surveillance and enforce robust guidelines to prevent compromising patient safety. Global harmonization of expedited approval processes, combined with transparent risk-benefit assessments, is essential to optimize the benefits of these programs while mitigating risks.

Keywords:

Fast Track Designation, Accelerated Approval, PRIME, Sakigake, Priority Review, Regulatory Affairs, Expedited Drug Approval, Public Health, Drug Safety



DRA-PM-030

Market Incentives and Policy Approaches for Orphan Drugs: A Global Review with Strategic Recommendations for India

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Background: Rare diseases, though individually uncommon, affect an estimated 6–8% of the global population. The development and accessibility of orphan drugs remain critical worldwide, particularly in developing countries like India. This review explores global regulatory frameworks, market incentives, and policy strategies with the aim of strengthening India's rare disease management ecosystem.

Objectives: This review aims to (1) Compare orphan drug regulations and market incentives across the U.S., EU and Japan (2) Analyse ethical and economic policy approaches that influence access to rare disease treatments (3) Assess India's current orphan drug landscape in the context of International best practices and (4) Propose strategic recommendations to strengthen rare disease management in India.

Methods: A literature search was conducted using pubmed and Google Scholar databases to gather academic articles, policy documents, and regulatory reports published between 2016 and 2025. Key policy frameworks were analyzed and synthesized narratively, focusing on drug regulations, market incentives, and access mechanisms for orphan drugs along with the comparison of India's orphan drug policy and rare disease management strategies to identify gaps, strengths, and areas for improvement.

Results: The U.S. leads in orphan drug approvals with over 1,000 approved therapies, supported by robust incentives like market exclusivity, tax credits, and priority reviews. The EU and Japan follow with more structured frameworks, including paediatric exclusivity and streamlined regulatory pathways. India, despite having over 70 million rare disease patients, lacks a dedicated orphan drug act, specialized regulatory mechanisms, and consistent reimbursement pathways. Financial barriers, limited post-marketing surveillance, and insufficient patient engagement persist.

Conclusion: India's rare disease policy environment requires urgent reform. This review recommends implementing legislative frameworks, enhanced collaboration, establishing a central orphan drug authority, enhancing financial and regulatory incentives, supporting local manufacturing, and improving patient-centric systems to bridge existing gaps and ensure equitable access to rare disease therapies in India.

Keywords: rare disease, orphan drug, FDA, EMA, PMDA



DRA-PM-031

The Role of Regulatory Agencies in Combatting Antimicrobial Resistance

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Background: Antimicrobial resistance (AMR) is a significant global health concern, driven by the overuse of antibiotics, circulation of poor-quality medicines, and inadequate regulatory oversight. This challenge is more acute in low- and middle-income countries due to weak regulatory systems and fragmented healthcare infrastructure. Strengthening regulatory authorities is essential to ensure the rational use of antibiotics, uphold drug quality standards, and improve access to effective antimicrobial therapies.

Aims & Objectives:

The objective is to review how regulatory authorities respond to AMR using policies, surveillance, harmonization, and expedited approvals. It also characterizes challenges and suggests how capacity in regulatory affairs in resource-poor environments can be made stronger.

Methods: This study is based on data from official reports by international health organizations, national regulatory frameworks, and relevant scientific literature. Key global initiatives such as the Global Antimicrobial Resistance and Use Surveillance System (GLASS), the Generating Antibiotic Incentives Now (GAIN) Act, and the National Antimicrobial Resistance Monitoring System (NARMS) were examined to explore and compare regulatory strategies in combating antimicrobial resistance.

Results: High-income countries have adopted fast-track approval processes and financial incentives to promote the development of new antibiotics. In contrast, low- and middle-income nations face significant challenges, including weak enforcement, limited surveillance systems, and insufficient global coordination. Key regulatory measures such as restricting over-the-counter antibiotic sales, implementing standard treatment guidelines, and strengthening post-marketing surveillance are essential to reduce misuse and control the spread of antimicrobial resistance.

Conclusion: Combating antimicrobial resistance (AMR) requires strong and coordinated regulatory systems. Both national and international authorities must work together to enforce



policies, ensure drug quality, and promote the responsible use of antibiotics. Adopting a unified One Health approach linking human, animal, and environmental health is vital to sustain effective antimicrobial practices and preserve the long-term efficacy of treatments.

Keywords:

Antimicrobial resistance, drug regulation, accelerated approval, WHO, FDA.



DRA-PM-032

New European Guidelines for Classifying Medical Devices and Software Qualification

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Background: The necessity for specific regulatory requirements has increased due to the rapid expansion of the software industry in the healthcare sector. In the European Union (EU), the phrases Software as a Medical Device (samd) and Medical Device Software (MDSW) are used. Software-based medical device categorization, qualification, and compliance have become more stringent since the Medical Device Directive (MDD) was superseded by the new EU Medical Device Regulation (MDR 2017/745) and In Vitro Diagnostic Regulation (IVDR 2017/746).

Objectives: To understand what is required for software items to qualify and be classified as risky under Rule 11 of the MDR, the Medical Devices Coordination Group (MDCG) in EU.

Methods: Study compares the present and former EU regulatory regimes and talks about the software device CE certification process.

Results: It emphasizes the involvement of Notified Bodies in the review process in addition to the new cybersecurity, usability, and data protection criteria (GDPR compliance) and basic non-conformities.

Conclusion: In order to ensure patient safety and legal compliance, the objective is to help developers, manufacturers, and regulatory specialists understand the steps required to introduce medical software products to the EU market.

Keywords: Software as Medical Device(samd), Medical Device Software(MDSW), Medical Device Directive(MDD)



DRA-PM-033

Nutraceutical Vaccines and the Evolving Global Regulatory Paradigm

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Background:

The development of nutraceutical vaccines represents a novel approach that integrates nutritional science with immunological benefits. These products, often derived from food-based bioactive compounds, aim to enhance immune response without relying solely on traditional pharmaceutical formulations. However, their classification remains unclear within most global regulatory systems, creating challenges in standardization, safety assessment, and market authorization.

Aims & Objectives:

This review explores the scientific foundation of nutraceutical vaccines, examines global regulatory approaches, and highlights key challenges in their classification and approval.

Methods:

A detailed literature search was carried out using scientific databases and official regulatory websites such as United States Food and Drug Administration (FDA), European Medicines Agency (EMA), Central Drugs Standard Control Organization (CDSCO), and a comparative analysis approach was applied to evaluate approval procedures, safety requirements, and post-market regulations for nutraceutical vaccines.

Results:

Nutraceutical vaccines face inconsistent global regulation, often falling between drug and supplement categories. While some authorities rely on intended use and composition, many lack clear guidelines, leading to challenges in product development, quality control, and market access.

Conclusion:

Nutraceutical vaccines offer significant potential in preventive healthcare. However, their effective integration into public health systems depends on the development of harmonized regulatory frameworks, including clear definitions, evaluation criteria, and labeling standards to ensure safety and foster innovation.

Keywords:

CDSCO, EMA, FDA, Global health policy, harmonization, Immune nutrition, Nutraceutical, vaccines, Regulatory challenges.



DRA-PM-34

The Need for Global Harmonization in Nutraceutical Regulations: A Critical Review of WHO, Codex Alimentarius, and ICMR Standards

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The growing consumer awareness of health and wellbeing is fuelling the rapid expansion of the global nutraceutical market. However there are major obstacles to product development market access safety assurance and consumer trust because of the absence of standardised worldwide rules. The current frameworks for the regulation of nutraceuticals set up by the Indian Council of Medical Research (ICMR) the Codex Alimentarius Commission and the World Health Organisation (WHO) are critically examine. The expanding importance of nutraceuticals and the critical role regulatory science plays in guaranteeing their efficacy; quality and safety. While ICMR creates national-level dietary and nutritional standards in India, Codex sets international food standards and labelling requirements and WHO offers broad guidelines centered on traditional medicines and health claims. Despite these initiatives there are still significant differences in post-market surveillance procedures, definitions, acceptable ingredients and claim substantiation. The study points out a crucial weakness in the lack of a unified regulatory framework which results in disparate product classifications, two regulatory loads, trade restrictions and weakened consumer protection in various geographical areas. This discrepancy restricts emerging countries like India's ability to compete internationally and stifles innovation. This examines the regulatory approaches of WHO, Codex and ICMR with a specific focus on India's nutraceutical regulations. The aim is to suggest a cohesive model that successfully balances public health with trade therapy enhancing regulatory uniformity, mutual recognition and global access to Indian nutraceuticals.



DRA-PM-035

India's Journey to Digital Therapeutics Regulation: Insights from the US and EU

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Digital Therapeutics (dtx) are scientifically validated software-based interventions that offer personalized and scalable healthcare solutions for the prevention, management, or treatment of a wide range of diseases. As their use expands globally, creating strong and consistent regulatory frameworks is essential to ensure that these technologies are safe and effective and protect patient data. This review compares how the United States, European Union, and India. The U.S. has clear pathways, such as the FDA's Software as a Medical Device (samd) and De Novo processes that support innovation while ensuring safety. In the EU, Germany digma model goes a step further by linking regulatory approval with reimbursement, encouraging the use of dtx in public healthcare systems, whereas India does not yet have a specific framework for dtx. Various agencies, such as the Central drug standards control (CDSCO), Ministry of health and family welfare (mohfw), and National digital health mission (NDHM), share responsibilities, resulting in fragmented regulation. Major issues include the absence of a risk-based classification system, a lack of specific guidelines for dtx, and the insufficient use of real-world evidence data. The study suggests that India should create a centralized regulatory body for dtx, implement health technology assessment (HTA), and uphold international clinical and data standards to address these issues. Such actions can support the establishment of a patient-focused, transparent, and flexible regulatory framework that encourages innovation and improves access to digital healthcare in India.



DRA-PM-036

Global Perspectives on the harmonization of Electronic information leaflets in the pharmaceutical industry

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Background: The pharmaceutical industry is rapidly transitioning from traditional paper-based Patient Information Leaflets (pils) to electronic labeling (e-labeling). E-labeling enhances patient safety, improves accessibility, and allows real-time updates. However, global implementation is inconsistent due to varying regulatory guidelines, data formats, and technological capabilities, creating challenges in harmonization and compliance.

Aims & Objectives: This review focuses on analyzing global e-labeling practices and exploring strategies for harmonization across regulatory frameworks. The objectives include evaluating current e-labeling regulations in regions such as the US, Europe, Japan, and India, identifying technological innovations in e-labeling, and proposing solutions to streamline digital labeling for global pharmaceutical use.

Methods: A comprehensive review was conducted on the electronic labeling frameworks adopted by international regulatory agencies, including the USFDA, EMA, PMDA, CDSCO, and others. The study examined data formats like SPL (Structured Product Labeling), epi (Electronic Product Information), XML-based systems, and QR code integrations. Challenges such as regulatory divergence, technological infrastructure, and data privacy were assessed alongside emerging digital tools like blockchain and AI-driven labeling systems.

Results: The review identified major regional differences in e-labeling implementation, including XML-based systems in the US and Japan, FHIR-based epi in Europe, and QR code-enabled labeling in India. Key innovations such as AI-assisted label generation, multilingual support, and blockchain-enabled traceability are driving the transition toward digital healthcare information. However, disparities in infrastructure, digital literacy, and regulatory acceptance remain significant barriers.

Conclusion: Harmonizing global e-labeling practices is essential for improving patient safety, enhancing regulatory efficiency, and supporting the digital transformation of healthcare. Standardized data formats, centralized digital repositories, QR code integration, and collaborative regulatory efforts are necessary to overcome current challenges. E-labeling represents a pivotal advancement toward safer, more transparent, and patient-centric pharmaceutical care.

Keywords: E-Labeling, Electronic Patient Information Leaflet (epil), Global Harmonization, QR Code, Structured Product Labeling (SPL), Fast Healthcare Interoperability Resources (FHIR), Regulatory Affairs, Digital Health, Blockchain in Pharmaceuticals.



DRA-PM-037

Biosimilar Adoption: Strategies to Overcome Barriers to Market Acceptance

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Widespread adoption of biosimilars might significantly improve healthcare access reduce treatment costs and promote system sustainability. The commercial awareness and public acceptance of biosimilars are still lacking despite the fact that they have been demonstrated to be clinically equal to their reference biologics. Regulatory ambiguity payer uncertainty patient opposition and physician reticence are some of the interconnected barriers that hinder the use of biosimilars.

Physicians often express concerns regarding the safety efficacy immunogenicity and interchangeability of biosimilars especially when it comes to replacing stable patients. Ignorance incorrect information and poor communication from healthcare providers are the main reasons why patients worry. Contradictory payment policies that limit incentives and ambiguous exchangeability and replacement regimes hinder adoption at the payer and pharmacy levels.

Regulatory barriers such as policy heterogeneity exclusivity extension and patent litigation complicate market entry and adoption. To overcome these challenges a comprehensive and collaborative approach is required. Important strategies include harmonizing international regulatory pathways providing medical staff with targeted training and education communicating in a clear and patient-friendly manner and changing policies to allow for automatic substitution when needed. Strong empirical evidence of safety and efficacy following switching formulary inclusion and financial incentives can all hasten the adoption of biosimilars in clinical practice. To build trust and guarantee long-term adoption stakeholder engagement that brings together regulators payers manufacturers doctors and patient advocacy groups is also essential.

The multifaceted nature of biosimilar adoption issues is emphasized in this review which also offers workable solutions to encourage wider acceptance. For biosimilars to reach their full potential in delivering affordable and accessible healthcare globally, a supportive environment will be required



DRA-PM-038

Regulatory Oversight of Parenteral Drugs: A Comparison Between the USA and GCC Regions

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Background: Parenteral preparations, such as injectables and sterile products, are vital for patients requiring immediate therapeutic effect. "FDA and GCC regulatory pathways ensure global standards, enabling safe, efficient market access and compliance for parenteral drug manufacturers worldwide." Their manufacturing demands rigorous sterility assurance, GMP compliance and stringent regulatory control due to the elevated risk of contamination and safety concerns.

Aims & Objectives: This study aims to compare the regulatory pathways for parenteral drugs under the FDA and GCC, with a focus on GMP compliance, sterilization requirements, approval processes, post-approval monitoring, and harmonization gaps.

Methods:

The study involved a detailed review of published literature, regulations from both USA and GCC. It compared core regulatory elements such as aseptic processing guidelines, dossier submission formats, facility inspections, and pharmacovigilance practices.

Results: The FDA follows an independent review model with stringent facility inspections and defined cgm standards, including aseptic process simulation. The GCC adopts a centralized approach, often relying on approvals from agencies like the FDA or EMA. Despite shared GMP standards, differences in documentation, language, and post-market surveillance highlight the need for regulatory alignment to improve approval efficiency and safety.

Conclusion: Though both regulatory bodies aim to ensure sterile drug quality and safety, procedural variations present barriers to global consistency. Strategies to address regulatory gaps and promote harmonization with global standards can streamline approvals and enhance sterile product safely compliance. Strengthening collaboration and aligning standards will benefit patient access and regulatory efficiency.

Keywords:

Aseptic Processing, FDA, GCC, GMP, Parenteral Preparations, Regulatory Pathways, Sterile Products,



DRA-PM-039

Supply Chain & Block-chain Regulation in Pharmaceutical Products.

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Background: The pharmaceutical supply chain is highly complex and strictly regulated, yet remains vulnerable to counterfeit medicines and data gaps. Traditional centralized tracking systems often struggle with limited transparency, fragmented data, and slow response times when product integrity is compromised. Blockchain technology, with its decentralized and tamper-resistant design, offers a way to strengthen product traceability and improve trust among stakeholders. At the same time, inconsistent regulations across countries and the challenge of aligning blockchain with existing systems remain significant barriers.

Aims & Objectives: This review explores how blockchain technology can be applied to strengthen regulatory oversight within the pharmaceutical supply chain. It examines current regulatory frameworks, highlights ongoing challenges, and discusses how harmonized policies could enhance traceability, patient safety, and compliance.

Methods: A targeted literature review was carried out using peer-reviewed research, international regulatory guidelines (e.g., FDA DSCSA, EMA serialization standards), and recent industry case studies. The review focused on four key themes: weaknesses in traditional supply chains, the role of blockchain-enabled serialization, cross-border regulatory inconsistencies, and emerging solutions. Case studies from Pfizer, Merck, Novartis, and IBM's Blockchain Traceability Solution were analyzed for real-world evidence.

Results: Evidence shows that blockchain can deliver end-to-end visibility, prevent counterfeit drug infiltration, and simplify regulatory audits through immutable data records. Early pilots demonstrate strong benefits when blockchain is combined with technologies such as IoT and AI for real-time monitoring. However, adoption continues to be slowed by high costs, a lack of global data-sharing standards, and misaligned regulations across regions. International efforts to harmonize supply chain regulations, including WHO-led initiatives, are emerging as key drivers for broader implementation.

Conclusion: Real-time pharmacovigilance represents the next evolution in drug safety. Its integration into regulatory frameworks and healthcare systems worldwide can significantly



enhance pharmacovigilance efficiency, enabling proactive responses to drug-related risks and improving public health outcomes.

Keywords: Pharmaceutical Supply Chain, Blockchain, Drug Traceability, Counterfeit Medicines, Artificial Intelligence, Regulatory Compliance.



DRA-PM-040

Emerging Trends in Smart Wearable Technologies Driving the Transformation of Personalized Healthcare

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Background: Today, the body speaks and technology listens. This has led to smart wearables that continuously monitor and interpret health signals in real time, transforming healthcare through constant tracking of health parameters. Devices like smartwatches, biosensors, and fitness trackers empower individuals and healthcare providers to monitor key health data anytime, anywhere, turning conventional systems into intelligent, real-time health management tools.

Objective: The present study explores emerging trends in smart wearables technologies driving the transformation of personalized healthcare.

Methodology: A literature search was conducted using scientific databases such as Scopus and pubmed to identify peer-reviewed journals, including review articles, case reports, and original research published between 2015 and 2025. Search strings combining keywords like “Wearable Health Devices” and “Personalized Healthcare” were used to filter relevant studies. The collected literature was then critically analyzed and thematically categorized under key areas: innovations, applications, challenges, and future trends in wearable health technologies.

Results: Initially, 3,181 articles were identified from Scopus and 7,563 from pubmed. After screening for the 2015–2025 publication period, 2,887 Scopus and 7,142 pubmed articles remained. Titles and s were then screened for relevance to the study objectives, and the most pertinent articles were thematically categorized. The corresponding references were added to their sections, providing structured, evidence-based insights into wearable health technologies in personalized healthcare.

Conclusion: Findings of the study reveal that wearable health technologies enable proactive, personized healthcare through real time monitoring and timely health insights. Despite all the challenges continuous innovation drives wearable technologies towards smarter, patient centered healthcare and ultimately enhancing global health outcomes.

Key Words: Wearable Health Technologies, Personalized Health Care, Patient Centered Care, Real Time Health Monitoring.



DRA-PM-041

Understanding UDI Compliance Under the USFDA Medical Device Framework

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Background: The Unique Device Identification System final rule (UDI Rule) requires device labels, typically the manufacturer, to unless the regulation specifies an exception or an alternative, include a unique device identifier (UDI) on device labels and packages.

Objectives: To provide device information to the Global Unique Device Identification Database (GUDID).

Methods: By a requirement that udis be listed on device labels, packaging, and, in some instances, direct labeling on devices, the system enhances adverse event reporting, streamlines recalls, avoids fake goods, and allows accurate device identification. Device information is centrally located in the Global Unique Device Identification Database (GUDID), ensuring transparency and accessibility.

Results: Study is to discuss the significance of data analytics, software applications such as EUDAMED, and new FDA rules on compliance time frames, particularly for Class I and disposable devices & also focus on standard UDI implementation issues, such as the necessity for integrated data management systems and misinterpretations of direct marking.

Conclusion: Provide an approach which involves efficient preparation, technology adoption, quality management integration, and continuous training to assist manufacturers achieve and maintain UDI compliance. To improve patient safety and efficiency in the rapidly evolving medical device environment,

Keywords: UDI, GUDID, AIDIC, QMS,



DRA-PM-042

Digital Therapeutics for Diabetes Management in India- Regulatory gaps and real world evidence.

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Background: In 2023, India records an estimated 101 million diabetes patients, and Type 2 diabetes continues to remain one of the most important public health issues. This creates a tremendous opportunity for Digital Therapeutics (dtx). Amid this rising burden, Digital Therapeutics (dtx)-evidence based software driven interventions is emerging as promising tools for individualized, technology enabled, scalable, and non-invasive disease management. Internationally, bluestar (Welldoc, USA) became the first FDA approved dtx for Type 2 diabetes, demonstrating clinical efficacy with hba1c reductions of 1.7 to 2.0 percent. In India, platforms like Wellthy Therapeutics and Fitterfly are gaining real world success as well. Still, India's lack of concrete policies regarding the regulation of digital therapeutics creates a crucial challenge hindering their effective integration into holistic healthcare systems.

Aims & Objectives: To analyze the potential of dtx for diabetes management in India and to evaluate existing regulatory gaps in India and measure them against global benchmarks. To create a roadmap for the governance, policy-making, and dtx integration into the Indian healthcare framework.

Methods: Google Scholar, pubmed, white papers, and even regulatory publications from WHO, dtx Alliance, and CDSCO were utilized for a systematic literature review. The FDA's Software as a Medical Device (samd) and Germany's Digital Health Applications (diga) were also reviewed for policy comparison alongside real-world data from Indian dtx platforms.

Results: Both Wellthy Therapeutics in India and bluestar, approved by US FDA, showcase improvements in patient engagement as well as decline in hba1c levels. There is no specific framework or pathway for dtx provided by CDSCO or NPPA in India. Compared to other frameworks, global ones focus more on the clinical evidence, data privacy, and reimbursement pathways. For India, this is however still very fragmented and underdeveloped. Initiatives like Ayushman Bharat Digital Mission (ABDM) offer great potential for dtx but lack regulatory accountability at this stage.

Conclusion: This is the right time for India to integrate dtx into the healthcare system legally and officially. In order to fully modernize diabetes care in India, there is a necessity to establish a regulatory framework anchored by CDSCO, which should ensure the clinical efficacy and safety of diabetes treatments through vigilant oversight while also safeguarding economical access to treatment and providing dependable insurance aid. This would foster innovation, investment, and improve India's international reputation by integrating pharmaceutical research with therapeutic application in MPCON 2025's theme.

Keywords:

Digital Therapeutics, Type 2 Diabetes, India, CDSCO, samd, Wellthy Therapeutics, bluestar, Regulation, dtx Approval



DRA-PM-043

The Future of Personalized Medicine: Regulatory Perspectives on Advanced Therapies

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Background:

Personalized medicine is poised to transform future healthcare by integrating genomics, artificial intelligence (AI), and digital tools. However, its widespread adoption depends on the evolution of regulatory frameworks, particularly in the USA and EU, to ensure safe, ethical, and equitable implementation across diverse populations.

Aims & Objectives:

This study aims to explore the future trajectory of personalized medicine through the lens of evolving regulatory frameworks in the USA and European Union. It focuses on how adaptive regulations, real-world evidence, and digital innovations like AI and digital therapeutics are shaping their integration into mainstream healthcare.

Methods:

A systematic review of literature was conducted using scientific databases, grey literature, and policy documents. The major areas of focus included genomic technologies, regulatory approaches, ethical issues, and emerging breakthroughs such as patient avatars, AI integration, and real-world evidence.

Results:

Personalized medicine has enhanced risk forecasting and treatment efficacy in cancer, cardiovascular, and orphan diseases. The USA FDA and the EU EMA have adopted regulatory strategies such as RMAT and ATMP pathways. Both regions support real-world evidence, precision pharmacovigilance, and conditional authorizations to drive innovation forward.

Conclusion:

The potential of personalized medicine lies in its seamless integration with AI, genomics, and real-time patient data. Evolution in regulatory policy across the USA and EU will be critical to



facilitating access to PM broadly, fairly, and ethically. Its success will be determined by robust collaboration between clinicians, innovators, and policymakers.

Keywords: Artificial Intelligence, ATMP, EMA, FDA, Genomics, Personalized medicine, Precision Health, Regulatory affairs



DRA-PM-044

UK Medical Device Regulators to Accept Extended EU Certificates.

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Background: The evolving regulatory landscape of medical devices in the United Kingdom following its departure from the European Union. It outlines the ongoing acceptance of extended EU CE certificates in Great Britain (GB) and examines how this aligns with the broader goal of ensuring continuous access to safe, effective, and high-quality medical technologies.

Objectives: To enhance regulatory harmonization, minimize supply disruption, and provide industry flexibility as the new UKCA framework is implemented.

Methods: Drawing on international guidance, including the World Health Organization's frameworks and the European Medical Device Directives, the article details classification systems, conformity assessment procedures, and the role of CE and UKCA markings.

Results: The responsibilities of UK regulatory bodies such as the Medicines and Healthcare products Regulatory Agency (MHRA), while addressing the transitional provisions, technical documentation standards, and conditions under which CE marking remains applicable.

Conclusion: Study highlights the transition period supports innovation and patient access while laying the foundation for a robust, future-ready medical device regulatory system in the UK.

Keywords: CE Certification, MDD, Mutual Recognition Agreements (MRA)



DRA-PM-045

Complexities in Medical Devices development and the plausible strategies to overcome these challenges

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Background: Over the past two decades, the landscape of medical devices has witnessed a consistent upsurge; however, there is a lack of unified classification system among the nations. Emerging medical devices introduce a host of novel challenges that evolve with the times, necessitating updated regulations to ensure effective oversight and management.

Aim & Objectives: The primary objective to understand the regulations pertaining to medical devices in the US, EU and India. Further identify the challenges in medical device development and recommend strategies to overcome the challenges.

Methods: A comparative analysis of research and review articles focusing on the complexities of various medical devices and their regulations. Primary source of Data – FDA, CDSCO and EU. Secondary source of Data – Scopus, pubmed, Google Scholar

Results: The study emphasizes on the challenges in various phases of Medical device development from pre-clinical, clinical and in approved and commercially available devices. Furthermore, the study highlights on identifying common challenges and recommend few strategies to overcome the same.

Conclusions: Addressing the disparities in classification of medical devices among the regulatory bodies poses an important challenge in developing medical devices.

Keywords: Central Drugs Standard Control Organization (CDSCO), clinical devices, EU Medical Device Regulation (MDR), FDA regulations, Preclinical devices.



DRA-PM-046

Evolving Regulatory Expectations for Biologics and Biosimilar – Global markets

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Background:

Biologics and biosimilars are transforming modern therapeutics by offering targeted, effective treatments for chronic and life-threatening diseases. Given their complexity and reliance on living systems for production, they require distinct regulatory oversight compared to traditional small-molecule drugs. Global regulatory agencies such as the FDA (USA), EMA (EU), and PMDA (Japan) have developed unique yet evolving frameworks for biologics and biosimilars, with increasing emphasis on comparability, post-market surveillance, and global harmonization.

Aims & Objectives:

This study aims to examine the evolution of regulatory expectations for biologics and biosimilars in global markets, evaluate challenges in biosimilar approval and commercialization, and offer strategic recommendations for navigating emerging regulatory landscapes.

Methods:

A qualitative, comparative approach analysed global regulatory frameworks, historical developments, and agency-specific guidelines. Data from FDA, EMA, PMDA, and ICH focused on approval pathways, interchangeability, and harmonization efforts to highlight evolving standards and regional differences in biosimilar regulation and oversight.

Results:

The analysis shows global regulatory pathways vary, especially in biosimilar interchangeability, surveillance, and trial requirements. While ICH and WHO promote harmonization, regional differences in definitions and data persist. Commercialization faces added hurdles from complex manufacturing, funding gaps, and ongoing patent-related challenges.

Conclusion:



Global regulatory expectations for biologics and biosimilars are continuously evolving. Harmonization efforts are advancing but need further alignment to facilitate market access, affordability, and therapeutic equity. Strategic collaboration among regulators, industry, and stakeholders is crucial to navigate regulatory complexity and promote biosimilar adoption.

Keywords: Biologics, Biosimilars, Comparability Studies, FDA / EMA / PMDA, Global Harmonization, ICH Guidelines, Interchangeability, Regulatory Expectations.



DRA-PM-047

Fecal Microbiota Transplantation: Current Advances, Safety Profile, and the Role of AI and Synthetic Microbiota

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Fecal microbiota transplantation (FMT) is discussed here along with its improved safety profile, procedures, and efficacy in treating gastrointestinal disorders, including recurrent *Clostridium difficile* infections (rcdi). The significance of FMT is highlighted by the growing need for innovative treatment alternatives in disorders linked to the microbiome, putting it at the top of personalised medicine. In this work, we highlight advancements in donor screening, preparation, and delivery methods that have helped FMT achieve these results through the application of transendoscopic tools and capsulized procedures. Additionally it takes into account the potential of artificial intelligence (AI) to expedite donor selection and treatment result prediction a discovery first made in this field as well as the potential of synthetic microbiota. The therapeutic use of FMT is still being carefully considered till then. This review emphasizes the urgent need for technique standardization, regulatory harmonization, and more research to overcome safety concerns and variability in patient outcomes. The authors outline the latest research and demonstrate how this paper is not only outlining that FMT has great potential as a new therapeutic strategy for microbiota-associated diseases it deserves consideration in future practices.



DRA-PM-048

Blockchain in Regulatory Affairs: Enhancing Transparency and Data Integrity

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Background: Maintaining data accuracy, transparency, and trust is a constant challenge in pharmaceutical regulatory processes. Traditional systems often fall short in ensuring data integrity and traceability, leading to inefficiencies and risks in compliance. Global regulatory agencies such as USFDA and EMA are exploring blockchain to improve data reliability and compliance oversight. Blockchain technology, with its decentralized and tamper-proof design, is emerging as a powerful tool to overcome these limitations.

Aims & Objectives: This study aims to explore how blockchain can be integrated into regulatory affairs to assess its role in strengthening data integrity, streamlining documentation, and improving real-time stakeholder collaboration

Methods: A detailed literature review was conducted to assess existing challenges in regulatory operations and evaluate blockchain's potential across multiple areas, including clinical trials, pharmacovigilance, supply chain monitoring, and electronic submissions. Case studies and pilot programs by regulatory agencies were also reviewed to understand practical implementation trends.

Results: Findings suggest that blockchain can significantly enhance data reliability and transparency. In clinical trials, it enables secure, time-stamped data entries. In the supply chain, it improves drug traceability and counters product falsification. Smart contracts further allow automated compliance with regulatory guidelines. Early-stage efforts by global regulatory bodies show promising acceptance of the technology.

Conclusion: Blockchain represents an innovative approach to modernizing regulatory affairs by creating systems that are more secure, transparent, and efficient. Although challenges like interoperability and regulatory standardization persist, industry-wide collaboration and pilot testing can pave the way for broader adoption.

Keywords: Blockchain, Data Integrity, Transparency, Clinical Trials, Regulatory Affairs, Pharmaceutical Supply Chain, Smart Contracts



DRA-PM-049

Bridging the Gap: Regulatory Challenges in Rare Diseases and Orphan Drug Development

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Background:

Rare diseases, though individually uncommon, affect over 300 million people globally. Historically neglected due to limited commercial viability, these conditions have gained increasing attention through regulatory frameworks designed to incentivize orphan drug development. Despite policy support and scientific advances, significant gaps remain in treatment availability. Equitable access to therapies continues to be a major challenge, particularly in low- and middle-income countries.

Aims & Objectives:

This study aims to critically evaluate global regulatory landscapes surrounding orphan drug development which identifies ongoing challenges such as inconsistent definitions, exploitation of incentives, and market access inequities, and propose actionable strategies for harmonized and patient-centered solutions.

Methods:

A comparative policy analysis was conducted, examining regulatory frameworks and incentive systems in the United States, European Union, and selected Asia Pacific countries like Japan and India. The study also analyzed challenges in clinical trial design, pharmacovigilance, market access, and post-marketing commitments, using peer-reviewed literature, official regulatory guidelines, and real-world case studies.

Results:

Findings reveal substantial divergence in rare disease definitions, approval pathways, and incentives. While regions like the U.S. and EU offer robust support systems, such as “salami slicing” which means breaking a rare disease into smaller subgroups to get multiple orphan drug approvals. It can help companies gain benefits repeatedly, even if the drug treats basically the same condition and “evergreening” which means companies make tiny changes to old drugs



(like tweaking the formula or delivery method) just to extend their patent and block competition. It's a way to keep making profits even after the original patent have expired. Access to orphan drugs remains uneven across geographies, and challenges in clinical trial design for small populations persist. Innovative frameworks such as adaptive trials, real-world evidence, and conditional approvals show promise, but lack uniform implementation.

Conclusion:

Bridging the regulatory gaps in orphan drug development requires global harmonization of definitions, coordinated regulatory frameworks, strengthened post-marketing surveillance, and greater patient engagement. Prioritizing ethical standards, affordability, and cross-border collaboration will be key to ensuring that life-saving therapies reach all rare disease patients regardless of location or economic status.

Keywords:

Health equity, orphan drugs, patient engagement, pharmaceutical policy, post-marketing surveillance, rare diseases, regulatory challenges.



DRA-PM-050

Regulatory Blind Spots in The Growing Market of Herbal Pharmaceuticals

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The market for herbal pharmaceuticals is expanding significantly on a global scale due to the growing use of natural and traditional treatments. However, this increase in demand also highlighted significant deficiencies in the current regulatory framework. National regulatory frameworks for herbal products are still uneven and frequently inadequate with no standardized requirements for post-market surveillance, safety, efficacy, or quality control. The lack of standardized international rules for herbal medications is a significant research gap that this review draws focus to. With little scientific support many nations permit market entrance based on historical or customary use. Regulatory blind spots include weak pharmacovigilance systems, herb-drug interaction, poor raw material uniformity, adulteration and contamination lack of batch-to-batch consistency and insufficient requirements for clinical studies. Furthermore, the risk of herb-drug interactions is increased by the widespread misunderstanding that "natural" means "safe," which encourages excessive consumption frequently without consultation from a physician. Ginkgo biloba and anticoagulant interactions are among the case studies that highlight the critical necessity for standardized safety monitoring and regulatory attention. These problems give rise to grave worries regarding product dependability and consumer safety. This review analyses identifies a basic regulatory inconsistency: many herbal products bypass rigorous clinical testing while synthetic drugs undergo stringent trials and it includes contrasting regulatory approaches of India, United States, European Union, China and WHO guidelines. It stresses the following critical needs: post-marketing surveillance, improved quality control procedures, globally harmonized regulatory requirements, and strong clinical trial frameworks for herbal medications.



DRA-PM-51

Labeling the Truth: How India and the US Govern Cosmetic Advertising and Consumer Protection

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This study tells about the consumer protection and cosmetic advertising environments in the US and India offering recommendations for both the legal frameworks and the actual experiences of consumers. The Drugs and Cosmetics Act 1940 and the Cosmetics Rules 2020 are a strong combination that regulates the cosmetics industry in India. These laws mandate registration clear labelling and strict prohibitions on misleading claims with penalties ranging from fines and product recalls to licence suspension and imprisonment for non-compliance. The Central Drugs Standard Control Organisation (CDSCO) is in charge of administration and consumer education programs are growing in importance.

The Consumer Protection Act of 2019 further increases consumer protection in India by Refreshing complaint processes and giving authorities the authority to punish producers promoters and advertisers for misleading advertising. In addition to ensuring compliance regulations focus providing consumers with information and channels for contesting deceptive advertising. The Fair Packaging and Labelling Act and the Federal Food Drug and Cosmetic Act are the two main laws in US Food and Drug Administration makes sure that all ingredients are listed correctly on cosmetics labels. The Federal Trade Commission also enforces laws against misleading advertising. The FDA now has more authority thanks to recent reforms but there are still gaps especially when it comes to clean beauty claims so consumers must figure out marketing terminology on their own.

Overall both nations share a common goal: protect public health and uphold consumer trust by ensuring that cosmetic advertising is fair transparent and evidence-based.



DRA-PM-052

Global Regulatory Trends in E-Labeling for Pharmaceuticals

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Background: Electronic labelling (e-labelling) is transforming how pharmaceutical information is communicated, replacing traditional paper-based labels that often lack real-time updates and multilingual accessibility. Regulatory agencies worldwide are exploring digital labelling frameworks, but global harmonization remains limited.

Aim and Objective: This review explores international regulatory approaches to e-labelling, highlights emerging trends, identifies key challenges, and offers strategic recommendations for effective implementation in the pharmaceutical industry.

Method: A narrative literature review was conducted using regulatory publications, peer-reviewed articles, and official documents from authorities such as the EMA, FDA, PMDA, MFDS, and TGA. Comparative analysis was applied across the EU, USA, Asia-Pacific, and select emerging markets.

Results: The EU (via EPI) and USA (via SPL) are leading structured efforts. Asia-Pacific countries show varied progress. Key trends include real-time updates, integration with electronic health records, mobile access, and use of technologies like blockchain. Challenges include fragmented regulations, limited infrastructure in some regions, data privacy issues, and digital literacy gaps among users.

Conclusion: Global e-labelling adoption is advancing but uneven. Strategic alignment, regulatory cooperation, and investment in digital infrastructure are essential. Pharma companies must prioritize patient-friendly, compliant e-labelling to stay aligned with evolving global standards.

Keywords: Digital Health, e-Labeling, epi, Global Regulations, Harmonization, Patient Safety, Pharmaceuticals, Regulatory Trends, SPL.



DRA-PM-053

International Regulatory Frameworks for Cosmetics: A Comparative Study of Standards and Regulatory Pathways

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Background: The global cosmetics industry is governed by diverse regulatory frameworks shaped by regional priorities, safety concerns, consumer preferences, and evolving scientific advances. While all jurisdictions aim to safeguard public health, differences in definitions, safety requirements, ingredient restrictions, labelling norms, and market access processes present significant challenges for stakeholders aiming for global compliance.

Aims & Objectives: This review aims to provide a comprehensive comparative analysis of international cosmetic regulations across the European Union (EU), United States (US), China, Japan, and ASEAN. The objective is to highlight the similarities, differences, recent regulatory updates, and emerging trends, thereby guiding stakeholders in achieving streamlined global market entry.

Methods: A narrative review approach was employed by analysing official regulatory texts, recent amendments (e.g., EU Regulation 2023/1545, mocra 2022 in the US, CSAR in China), and international harmonization initiatives like ICCR and ASEAN directives. Comparative tables and graphical models were used to illustrate regulatory distinctions in pre-market requirements, GMP compliance, safety evaluations, and animal testing policies.

Results: The EU enforces strict safety and labelling rules; China emphasizes pre-market registration; the US modernizes via mocra. Japan distinguishes quasi-drugs. Trends include digital compliance, sustainability, and allergen transparency.

Conclusion: Diverse regulatory landscapes compel cosmetic firms to adopt robust, adaptive compliance strategies. Harmonization efforts, digital tools, and proactive regulatory intelligence are key to overcoming trade barriers and fostering innovation while maintaining global consumer safety and trust.

Key words: Cosmetic safety standards, Global compliance requirements, Good Manufacturing Practices (GMP), Product Information File (PIF), Marine-derived bioactive, Sustainability in cosmetics



DRA-PM-054

Comparative Study of Drug Approval Process: Insights from USFDA, EMA, and CDSCO

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Background: International drug development and market access are heavily reliant on the ability to transit varied regulatory systems. United States Food and Drug Administration (USFDA), European Medicines Agency (EMA) and Central Drug Standard Control Organization (CDSCO) are the prime agencies responsible for regulating drug approvals in large markets. Though these agencies share common objectives of providing drug safety and efficacy, they vary in terms of approval periods, submitting formats, and post marketing obligations.

Aims & Objectives: The research intends to comparatively review the drug approval procedures of USFDA, EMA and CDSCO in terms of review routes, timelines, documentation needs, and pharmacovigilance practices. It also attempts to determine challenges and opportunities for harmonization in regulatory affairs.

Methods: Systematic review was performed by reviewing official guidelines, regulatory texts, and published literature of respective agencies. Procedural steps, timelines, electronic submission systems, and post-marketing surveillance data were gathered and contrasted. Visual aids such as flowcharts and comparative tables were created for differences to be seen clearly.

Results: The review indicates that USFDA and EMA have established electronic submission systems and strictly defined timelines (around 10-12 months and 7 months respectively for routine reviews). The approval process of CDSCO is longer (12-18 months) with varying timelines due to committee reviews are semi-digitization. The agencies all employ the ICH Common Technical Document (CTD) format but vary in electronic submission maturity. Post-marketing monitoring is also not uniform, with USFDA and EMA having active pharmacovigilance programs, while CDSCO is progressive though less uniform.

Conclusion:

Disparities between regulatory processes underpin the necessity of increased global harmonization simplify drug approval and increase patient access. Rapid uptake of electronic submission and uniform pharmacovigilance structures, especially from new regulatory authorities, will enhance regulator effectiveness and conformity.

Keywords:

Drug Regulatory Affairs, USFDA, EMA, CDSCO, Drug Approval Process, Pharmacovigilance



DRA-PM-055

Learning from the Giants: Strategic Policy Shifts to Boost India's Pharma Autonomy

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Background:

India's "pharmacy of the world" faces vulnerabilities due to overdependence on foreign Active Pharmaceutical Ingredients, medical equipment, and raw materials. COVID-19, US tariff hikes, and global trade uncertainty have exposed these risks.

Objective:

This study aims to examine the economic and regulatory implications of India's pharmaceutical import dependence and to propose creative, long-term policy solutions for enhancing domestic resilience and self-reliance.

Methodology:

We undertake a comparative analysis of pharmaceutical policy strategies employed by global leaders to bolster domestic manufacturing and exports, Production-based incentives, export subsidies, and strong R&D support that have cemented its API dominance from China, Regulatory flexibility, tax incentives, and heavy investment in medical technology R&D that fuel its export strength from United States and a quality-first approach with regulatory harmonization and a focus on strategic autonomy from Europe. These models are analyzed to identify best practices and benchmark India's current policy environment.

Results:

Our analysis reveals critical policy gaps in India's pharmaceutical ecosystem, including regulatory inefficiencies, limited incentives for domestic API and device manufacturing, and a lack of alignment with international quality standards. Comparative insights suggest that targeted interventions—such as fast-tracking regulatory approvals, incentivizing domestic production, and adopting globally harmonized quality benchmarks—could significantly reduce import reliance and foster innovation.

Conclusion:

India must adopt integrated strategies to build pharmaceutical sovereignty, enhancing industry resilience, reducing import dependence, and enhancing innovation and self-reliance manufacturing. These steps are crucial for long-term drug security and global pharmaceutical market leadership.

Keywords: Pharmaceutical policy, Import dependency, Drug regulatory affairs, Global pharma comparison, Policy incentives, India pharmaceutical industry, Comparative Analysis

Category 3

Pharmaceutical Analysis and Quality Assurance

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PA-QA-001

LC-MS Guided Screening of Bioactive Metabolites from Probiotic Bacteria Isolated from Honey: In-vitro and In-silico Assessment Against *Vibrio cholerae*

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Background:

Probiotic products are increasingly popular due to their potential health benefits, with recent research emphasizing the discovery of new probiotic bacteria that possess natural antimicrobial properties. Honey, known for its inherent antimicrobial activity, has emerged as a promising natural source for isolating beneficial microorganisms.

Aim & Objectives:

The present investigation was designed to isolate probiotic bacterial species from local honey samples and assess their bacteriocin production and antimicrobial activity against *Vibrio cholerae*. Additionally, the study aimed to identify the bioactive components present in the bacteriocin and evaluate their interactions with cholera-related proteins using molecular docking techniques.

Methods:

Gram-positive bacilli were successfully isolated from honey and identified through morphological, biochemical, and molecular characterization. The bacteriocin extracted from these isolates was analyzed using LC-MS/MS with esi mode, utilizing a mobile phase of 0.1% formic acid in water and acetonitrile (ACN) with gradient elution on a C18 column. The secondary metabolites were detected at 280 nm using a PDA detector. A total of 64 bioactive compounds were identified, of which 8 high-intensity compounds were selected for molecular docking studies using Biovia Discovery Studio on PDB proteins 6EHB and 3GBG.

Results:

The isolated gram-positive bacilli demonstrated notable probiotic potential, with the bacteriocin exhibiting significant inhibitory activity against *Vibrio cholerae*. LC-MS/MS analysis revealed 64 bioactive compounds, among which Cyclo, 2,3,5,7-tetramethoxy-9,10-dihydrophenanthrene, Diboal, Trans-4-hydroxy-L-proline, and Trans-cinnamic acid displayed the highest binding energy during molecular docking, indicating strong anti-cholera activity.

Conclusion:

This study establishes honey as a rich source of probiotic bacteria capable of producing bacteriocins with potent antimicrobial effects against *Vibrio cholerae*. The identified bioactive compounds, particularly those with high docking affinities, show promising potential as natural therapeutic agents for combating cholera.

Keywords:

Vibrio cholerae, probiotic, LC-MS/MS, molecular docking, ompu, toxt.



PA-QA-002

Green FTIR Approach for the Estimation of Pinaverium Bromide in Pharmaceutical Tablets

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Background

Pinaverium bromide is a calcium channel blocker used primarily to manage functional gastrointestinal disorders. It works by restoring the normal contraction process of the bowel, alleviating symptoms such as abdominal pain, bloating, and irregular bowel movements. The drug's mechanism of action involves inhibiting calcium influx into smooth muscle cells, reducing spasms, and improving gastrointestinal motility. Innovative infrared spectroscopic methods have been developed to quantitatively analyze pinaverium bromide, enabling its accurate determination in bulk and marketed formulations. These methods offer a robust, non-destructive, and green approach to drug analysis, aligning with eco-friendly principles. Analytical methods were rigorously validated according to International Council for Harmonisation (ICH) guidelines, ensuring reliability, precision, and accuracy in detecting pinaverium bromide across various applications.

Aim & Objectives:

The method aims to quantify the Pinaverium bromide by eco-friendly method. To Establish a reliable and reproducible Fourier Transform Infrared (FTIR) spectroscopy method for the quantification of pinaverium bromide in pharmaceutical tablet. To minimize the use of hazardous solvents and reagents in the analysis process, aligning with green analytical chemistry principles.

Method:

Accurately weigh a specified amount of pure Pinaverium Bromide and prepare a series of standard solutions by mixing with potassium bromide (kbr) in appropriate ratios. Typically, 1-2 mg of the drug is mixed with 100-200 mg of kbr to form a fine, homogeneous powder. The tablet form of Pinaverium Bromide and kbr in a 1:100 ratio was scanned.

Results:

The proposed methods have been effectively developed and validated for the quantification of pinaverium bromide in both solid bulk and dosage forms. The high recovery rates observed during the analysis of pinaverium bromide demonstrate the methods have a strong accuracy. Additionally, the methods exhibit exceptional repeatability and consistent intermediate precision.

Conclusion:

The proposed Fourier Transform Infrared (FT-IR) spectroscopic methods were demonstrated to be specific, reliable, and valid, making them suitable as general techniques for the qualification of various solid drug formulations, including tablets, capsules, and powders.

Keywords: Pinaverium bromide, gastrointestinal, FT-IR



PA-QA-003

Sophisticated Analytical Studies of Jawarish Shahi: A Classical Unani Medicine

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Traditional Unani medicine emphasizes holistic healing through natural formulations. Jawarish Shahi, a classical polyherbal Unani preparation, is traditionally used for its tonic, digestive, and neuroprotective benefits. This study aimed to scientifically evaluate Jawarish Shahi using modern analytical techniques. The marketed formulation underwent organoleptic, phytochemical, and biochemical tests. Advanced methods—Fourier-Transform Infrared Spectroscopy (FTIR), Gas Chromatography-Mass Spectrometry (GC-MS), and High-Resolution Liquid Chromatography-Mass Spectrometry (HR-LCMS)—were used to identify and characterize its bioactive compounds. Phytochemical screening revealed the presence of alkaloids, glycosides, flavonoids, tannins, saponins, and fixed oils. FTIR confirmed functional groups such as alcohols and ketones, while GC-MS and HR-LCMS detected compounds with neuroprotective and antioxidant activity. Biochemical analysis showed essential elements like zinc, iron, and sodium, but also trace levels of mercury and arsenic, indicating the need for safety validation. Overall, Jawarish Shahi demonstrates potential in managing neurological disorders like depression, aligning with Unani principles. Further toxicological studies are recommended to ensure its safety and efficacy.

Keywords:

Unani medicine, Jawarish Shahi, phytochemical analysis, FTIR, GC-MS, HRLCMS, depression, herbal formulation



PA-QA-004

Development Of Method for Analysis of Selected Poisoning Substances

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Background:

Intentional or accidental poisoning presents significant forensic and public health challenges. Accurate identification of toxins in biological samples is essential for prompt treatment and legal purposes. Conventional qualitative methods, such as functional group analysis and colorimetric tests, lack sensitivity and specificity. Advanced techniques like mass spectrometry and RP-HPLC improve detection but require further clinical refinement.

Aims & Objectives:

This study aims to detect toxins in poisoned patients using RP-HPLC at a tertiary hospital, gather regional data, enhance poison information services, and assess RP-HPLC's diagnostic accuracy.

Methods:

A prospective study was conducted at JSS Hospital, Mysuru. Poisoned patients in the Emergency and ICU wards were enrolled after informed consent. Data on demographics, poison type, route, and intent were collected. Blood samples (5 ml) were centrifuged, and serum was analysed via RP-HPLC using ACN-based extraction. Severity was assessed using the Glasgow Coma Scale (GCS) and Poison Severity Score (PSS). Data were documented and statistically analysed.

Results:

The study developed RP-HPLC methods to detect toxins like cypermethrin, dimethoate, and digoxin in serum, highlighting diagnostic value. Among 120 cases, 62.5% were aged 17–35, and 59.17% were female. Intentional poisoning made up 75.8%, mainly due to pesticides (48.33%), followed by acetaminophen and benzodiazepines. Moderate GCS was seen in 58.33%, with PSS showing 67.5% moderate, 26.6% severe, and 1.66% fatal cases.

Conclusion:

Poisoning, particularly among those aged 17–35, is rising, with most cases intentional. Organophosphate pesticides are common in rural areas, while paracetamol dominates urban cases. Both can cause severe or fatal outcomes if untreated. The trend highlights the need for stricter regulations, public awareness, and timely medical access.

Keywords:

Poisoning, Clinical Toxicology, Poison Information Services, Analytical Techniques



PA-QA-005

Development and Validation of a Reversed-Phase HPLC Method for Quantifying Chrysin and Curcumin in Bulk Drug and Pharmaceutical Formulation.

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Background:

Curcumin and Chrysin are two well-known drugs which have anti-inflammatory, anti-oxidant, anti-cancer, and neuro protective activity respectively. But when used in combination they are known to be potent anticancer agents. It was studied that a combination of Chrysin and Curcumin has shown promising anticancer activity in breast cancer cells in laboratory studies according to the literature survey. They may inhibit the growth of breast cancer cells and induce apoptosis (cell death) in certain breast cancer cell lines. In the current study, we have focused on development of HPLC method for the simultaneous estimation of Curcumin and Chrysin in pharmaceutical dosage form and its validation using various parameters according to ICH guidelines.

Aims & Objectives:

To establish a precise, accurate, and robust RP-HPLC method addressing the need for reliable simultaneous analysis of chrysin and curcumin in bulk pharmaceutical active ingredient and dosage form.

Methods:

Curcumin and Chrysin were obtained as gift sample from the industries. The instruments used for our study were Shimadzu UV- 1900i with Lab Solutions software and Agilent Technologies' 1220 Infinity II LC (High Performance Liquid Chromatography).

Results:

The method carried out by HPLC was found linear for both Curcumin and Chrysin in the concentration range of 2-10 µg/ml with correlation coefficients (r^2) of 0.9998 and 0.9993 for 358nm respectively. Ruggedness, robustness, and precision data showed %RSD <2%. Accuracy was observed within the range of 90% to 110%.

Conclusion: The HPLC method developed is reliable, exhibiting simplicity, precision, specificity, and sensitivity for the simultaneous estimation of Curcumin and Chrysin in bulk form.

Keywords: Chrysin, Curcumin, ICH guidelines, HPLC.



PA-QA-006

Validated RP-HPLC method for the estimation of Nortriptyline hydrochloride in marketed formulation: Evaluation by green and white tools

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Background:

Analytical method development and validation are essential to ensure the quality, efficacy, and safety of pharmaceutical formulations. The green and white analytical tools were incorporated for the first time for the proposed method and these principles will enhance environmental sustainability and method reliability.

Aims & Objectives:

The main objective of the study was to develop and validate Nortriptyline hcl in the marketed formulation by using Reverse-phase High-Performance Liquid chromatography (RP-HPLC) as per ICH Q2R1 guidelines. Additionally, by utilizing a green and white algorithmic tool, the effectiveness of the suggested analytical method was compared with two previously published approaches via algorithmic tools such as Analytical greenness metric approach (AGREE), Modified green analytical procedure index (mogapi), Blue applicability grade index (BAGI), Red analytical performance index (RAPI), and Red Green Blue (RGB).

Methods:

Chromatographic separation was performed using a Shimpack solar C18 column (4.6 x 250 mm, 5 μ m) with a mobile phase consisting of 90% methanol and 10% sodium acetate buffer (ph adjusted to 5.0 with glacial acetic acid), with the flow rate 1.0 ml/min, and detected at 239 nm. The method's greenness and whiteness were evaluated using algorithmic tools.

Results:

Nortriptyline hcl was eluted at a retention time of 3.52 min with a total run time of 6 min. The method demonstrated linearity in the concentration range of 1–10 μ g/ml, with a regression coefficient (R^2) of 0.9991. The method was successfully applied for the assay of Nortriptyline hcl in marketed tablet dosage forms.

Conclusion:

The developed RP-HPLC method is accurate, precise, and eco-friendly compared to reported methods. It meets the greenness and whiteness criteria and can be effectively applied for the routine analysis of Nortriptyline hcl in pharmaceutical formulations.

Keywords: AGREE, mogapi, BAGI, RAPI, RGB.



PA-QA-008

Development and validation of cost-effective UV spectrophotometric methods for quantitative analysis of Abametapir

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Background:

Abametapir is a topical pediculicide used in the treatment of head lice infestations. Despite its therapeutic relevance, standardized analytical procedures for its routine quantification remain limited.

Aims & Objectives:

This study focuses on designing and validating simple, economical UV spectrophotometric methods to quantify Abametapir in bulk form, suitable for routine laboratory application.

Methods:

Four spectrophotometric approaches Direct Absorbance, Derivative Spectrophotometry and Area Under Curve (AUC) methods have been developed and rigorously validated as per ICH Q2(R1) guidelines. Analytical parameters including linearity, precision, accuracy, limit of detection (LOD) and Limit of Quantification (LOQ), robustness were evaluated across a concentration range of 2–10 µg/ml.

Results:

All methods displayed excellent linearity with correlation coefficients (r^2) > 0.999. The AUC method showed superior sensitivity, with an LOD of 0.0184 µg/ml and high precision (%RSD < 0.04). Recovery rates ranged from 98% to 102%, indicating robust accuracy. Method robustness remained consistent despite minor modifications in wavelength and solvent composition.

Conclusion:

These UV-based techniques are reliable, reproducible, and highly suited for routine quality control of Abametapir, especially in resource-constrained environments. They offer practical alternatives to chromatographic systems for educational and small-scale pharmaceutical laboratories.

Keywords:

Abametapir, UV Spectrophotometry, Method Validation, Head Lice Treatment, AUC, ICH Q2(R1), Routine Analysis.



PA-QA-009

Stability evaluation of marketed brands of amoxicillin trihydrate and potassium clavulanate tablets at various conditions

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Background: The fixed dose combination (FDC) of amoxicillin (AMO) and clavulanate potassium (CLA) is a widely prescribed medicine to combat bacterial infections. However, this FDC faces stability challenges related to humidity and temperature, which can impact the efficacy and shelf-life.

Aims & Objectives: To perform an *in vitro* stability comparison study of leading marketed brands of amoxicillin and potassium clavulanate tablets (FDC) coded Brand 1, Brand 2 (CLAMP obtained from Dr Reddy's Laboratories), Brand 3, and Brand 4.

Methods: The stability was conducted at different stability conditions such as room temperature, air conditioner condition (22-25°C), refrigerator condition (2-8°C), ICH intermediate condition (30±2°C/ 65±5% RH), and at ICH accelerated conditions (40±2°C/ 75±5% RH). The time points for the study were 0, 3, and 6 months. The *in vitro* parameters were physical appearance, hardness, thickness, friability, weight variation, disintegration, dissolution, % moisture content, and % assay. The procedures for the following studies were followed as per IP 2022.

Results: Visual inspection of the tablet for each brand showed that the shape of all brands was oval, with no capping, mottling, or fungal growth at all time points and at all conditions. The hardness of tablets of all brands is within the acceptance limits of 4-10kgf. In the case of Brand 2, the hardness was less than that of other brands at all conditions and at all time points. The friability study showed negative results, possibly from moisture absorption during the testing process. The weight variation of tablets of all brands were within the acceptance limits, the individual weight did not deviate from the average weight by ± 5%. The disintegration test showed that tablets of all brands passed the test and disintegrated within 30 minutes. In case of Brand 2, it disintegrated within 10 min earlier than other brands at all conditions at all time points. The % moisture content study showed that the moisture content in the tablet of all brands was within the acceptance limit of less than 10%. The dissolution test showed that tablets of all brands passed the test and released more than 80% of the drug within 30 minutes, which is under the acceptance limits. In the case of CLAMP, tablets released more than 80% of the drug within 10 min, earlier than other brands in all conditions at all time points. The % assay study showed that the amount of both drugs in tablets of all brands was within acceptance criteria IP (% assay not less than 90% and not more than 120%).

Conclusion: The stability study of the marketed tablets of FDC containing amoxicillin and clavulanate potassium did not show any significant degradation of the drug. All the studied brands passed all the quality control tests specified as per the India Pharmacopoea after storage at various stability conditions including the accelerated stability conditions. A key observation



in the study was that the CLAMP (Brand 2) tablets showed a release of more than 80% of the content within 10 minutes, which could be linked to the lesser hardness and the earlier disintegration. This earlier release could benefit in an earlier bioavailability of the medication to the patient.

Funding: This research was funded by Dr. Reddy's Laboratories Ltd, Hyderabad, Telangana.

Keywords: Amoxicillin, clavulanate potassium, stability, moisture content, drug release



PA-QA-010

An Antibiotic-Free Strategy: In Vitro Synergistic Bactericidal Action of Berberine-Clove Oil Nanoemulsion on *Helicobacter pylori*

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Background: *Helicobacter pylori* (H. Pylori) infection remains a significant challenge due to increasing antibiotic resistance and the low bioavailability of conventional therapies at the gastric mucosal site, leading to treatment failures and peptic ulcer disease and gastric cancer risk. **Objective:** This study investigates a novel strategy to enhance H. Pylori eradication by combining berberine, a natural alkaloid with known antimicrobial properties, with clove oil, a potent essential oil, within a nanoemulsion delivery system. **Methodology:** An oil-in-water nanoemulsion was developed using clove oil as the primary oil phase to encapsulate berberine, which is hydrophobic in nature. The formulation was characterized for key physicochemical attributes including particle size, polydispersity index, and zeta potential, confirming its nanoscale dimensions and stability. The entrapment efficiency of berberine within the clove oil nanoemulsion was also determined. The in vitro bactericidal activity and synergistic potential of the berberine-loaded clove oil nanoemulsion against H. Pylori were evaluated using a checkerboard microdilution assay. **Result:** The optimized berberine-clove oil nanoemulsion exhibited favourable characteristics for drug delivery, including small, uniform particle sizes and good stability. The bactericidal assays demonstrated a significant synergistic effect between berberine and clove oil when delivered in this nanoemulsion format. The combination effectively reduced the minimum inhibitory concentrations of both agents against H. Pylori, leading to enhanced bactericidal activity. **Conclusion:** These findings suggest that a berberine-clove oil nanoemulsion holds substantial promise as an innovative and effective approach for H. Pylori eradication, offering a potential solution to combat resistance and improve therapeutic outcomes.

Keywords: *Helicobacter pylori*, Nanoemulsion, Antibiotic resistance, Antimicrobial Activity, Berberine.



PA-QA-011

Quantification of MSG via Green FTIR Spectroscopy

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Background: Monosodium glutamate (MSG) is a widely used flavour enhancer, first isolated in 1908 by Japanese scientist Kikunae Ikeda from the seaweed *Laminaria japonica*. It appears as a white, odourless crystalline powder with a molecular weight of 187.13 and is highly soluble in water. MSG is the sodium salt of L-glutamic acid, a non-essential amino acid naturally found in foods such as Parmesan cheese, tomatoes, mushrooms, meats, and vegetables. It is also synthesized in the human body and plays a vital role in metabolism. Commercial production of MSG involves fermentation of starch, corn sugar, or molasses. Purified to at least 99% glutamate is labelled as monosodium glutamate, whereas lower purity variants are classified as hydrolysed protein products (HPP). An alternative processing method utilizes protease enzymes, which, in some cases, may not require specific labelling in food applications. The detection and analysis of MSG have been optimized using green, non-destructive techniques that align with sustainable analytical practices. These methods have been rigorously validated following International Council for Harmonisation (ICH) guidelines, ensuring precision, accuracy, and reliability in the identification of MSG across various applications.

Aim: The method aims to quantify the Monosodium Glutamate in the sample by eco-friendly method.

Method: The study materials include Manchow Soup and Pasta Masala purchased from commercial markets in Mysore. The absorbance data obtained from Fourier Transform Infrared (FTIR) spectroscopy were analysed using labsolutions software, with monosodium glutamate (MSG) identified as the primary component.

Results: The developed methods have been successfully established and validated for the quantification of monosodium glutamate. To assess the similarity of raw materials, food additives, and auxiliary ingredients in various commercially available seasonings, Fourier Transform Infrared (FTIR) spectroscopy was utilized by analysing their absorbance patterns.

Conclusion: The developed and validated methods provide a reliable and efficient approach for the quantification of monosodium glutamate across various applications. The use of Fourier Transform Infrared (FTIR) spectroscopy enables a precise comparison of raw materials, food additives, and auxiliary ingredients in commercially available seasonings by analysing their absorbance patterns. These techniques align with green analytical principles, ensuring accuracy, reproducibility, and sustainability in MSG detection and characterization.

Keywords: Monosodium glutamate, FTIR, eco-friendly.



PA-QA-001

A Novel Chiral Isoquinoline Derivatives: Synthesis, Separation and Identification of Individual Enantiomers for Anti-cancer activity

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Background: CDK4/6 inhibitors are a substantially current menage of drugs that are used to treat hormone-receptor-positive, HER2-negative breast cancer. These inhibitors interfere with the mechanism through which breast cancer cells divide and grow by shepherd cyclin-dependent kinase 4 and 6 (CDK4/6). The hormones estrogen, progesterone, or both play key role in breast cancer development. Herceptin a protein that stimulates cancer cell proliferation, has been found to be absent in HER2-negative tumors.

Aim & Objective: On the report of review literature related to the proposed work, it focuses uniquely on the synthesis of novel isoquinoline components, as well as the exploration of commercially available isoquinoline derivatives/drugs. Proposed project is related to the drug development of chiral isoquinoline analogues.

Methods: It focus on redesign and synthesis of chiral isoquinoline compounds, evaluation of anticancer activity. Separating the racemic mixture of active molecule by HPLC methods. Further, cell line studies of individual enantiomers and analytical method development of chiral molecules.

Results: B-04 & B-06 molecules shows the good activity against marketed drug Palbociclib. So these two molecules are furtherly taken for separation and evaluation. Conclusion: We anticipate a one or more molecules of them would emerge as potential anticancer agent. Such molecule will be taken further for optimization to get improved efficacy.

Keywords: CDK4/6 inhibitors; HER2-negative; isoquinolines; anti-cancer activity; Enantiomers.



PA-QA-013

GC-FID Based Simultaneous Analytical Method for Residual Solvent and Validation

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Background:

The main goal of this research is to develop a simple, sensitive, and fast method for determining the Methanol, Ethanol, 1-propanol, and 2-propanol in the raw materials used in the manufacturing of OTC products, as most of the methods applied require considerable time.

Aims & Objectives: Presented here is a simple and fast Gas Chromatography- Flame Ionization Detector (GC-FID) method for simultaneous detection of methanol, ethanol, 1-propanol, and 2-propanol in the raw materials using ZB-624 column (30m* 0.53mm* 3.0µm) using 1-butanol as an internal standard. Developing a method to quantify methanol, ethanol, 1-propanol, and 2-propanol in raw materials.

Methods: The flow rate was 1.0ml/min, the column oven temperature was programmed to 50°C, held for 3 mins and then 20°C/min to 200°C, hold for 8 mins. The Detector (FID) temperature was 230°C, and the injection volume was 0.2µl with a split ratio of 5:1.

Results: The retention times of Methanol, Ethanol, 1-propanol, and 2-propanol were found to be 8.602mins, 9.323mins, 10.56mins, and 9.744mins along with 1-butanol having the retention time of 11.865mins. The relative standard deviation was found to be below 5% as per ICH Q3C R8 and was found to be 3.867131, 4.830157, 2.684971, and 2.183576 for Methanol, Ethanol, 1-propanol, and 2-propanol respectively.

Conclusion: The method was validated for Repeatability, specificity, Linearity, Limit of Detection, and Limit of Quantification and adhered to ICH Q3C R8 guidelines.

Keywords: Gas Chromatography, Flame Ionization Detector, Residual Solvents, Methanol, Ethanol, 1-propanol, 2-propanol, Analytical method development, ICH guidelines.

PA-QA-014

Exploring Nurses' Perception on Patient Safety Culture

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Background:

Medication errors represent a significant threat to patient safety. Nurses play a pivotal frontline role in patient care through medication administration and monitoring.

Aims & Objectives:

This study explored nurses' perceptions related to various dimensions of patient safety culture and its practice in a tertiary care hospital setting.

Methods:

Descriptive, cross-sectional study enrolling 295 nurses with minimum one year of work experience was conducted at a multi-disciplinary tertiary care hospital in Southern India. After Institutional Ethical clearance, data was collected via structured, self-administered questionnaire shared to participants through social chat applications. Link was shared after personally interacting with nurses to explain study purpose and take their informed consent. Questionnaire consisted of demographics and AHRQ(Agency for Healthcare Research and Quality)'s Hospital Survey on Patient Safety Culture questions. Descriptive statistics were used to analyse data. Bivariate associations were explored using Chi-square with significance set at $p < 0.05$.

Results:

Participant pool was predominantly female, professionally qualified, and actively involved in patient care. Majority respondents reported no patient safety incidents, suggesting robust intra-unit communication and institutional learning across experience levels. Nurses cited lack of time, inadequate staffing, absence of standardized protocols, and perceived primary physician responsibility as key execution challenges. Respondents' educational background did not significantly affect their perceptions of patient safety dimensions. Authors noted that workload stress was not directly perceived as compromising safety culture.

Conclusion:

Nurses demonstrated strong foundational patient safety awareness and positive intra-unit collaboration suggesting on-the-job culture and institutional safety practices shape safety attitudes more than academic qualification. Addressing vulnerabilities by institution-wide policy, training, and communication reforms can foster a safer, more open, and adequately staffed healthcare environment. Further qualitative insights would be valuable to explore hidden workload stressors or adaptive behaviors among nurses.

Keywords: Error Reporting, Healthcare Quality, Nurses, Tertiary Care



PA-QA-015

Green and white validated RP-HPLC method for the estimation of Posaconazole in its pharmaceutical formulation

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Background: Developing and validating an analytical method is crucial to guarantee the well-being, effectiveness, and quality of pharmaceutical product. For the first time, green and white analytical tools are incorporated to assess the environmental benign and throughputness of developed and validated Reverse-phase High-Performance Liquid Chromatography (RP-HPLC) for posaconazole in its marketed formulation.

Aims & Objectives: The primary aim of the current research was to develop and validate an eco-friendly RP-HPLC method for the estimation of Posaconazole in its marketed formulation as per ICH Q2R1 guidelines. Further, the proposed analytical method Eco-friendliness and Performance was compared with two reported methods using green and white algorithmic tools such as Analytical Greenness metric approach (AGREE), Modified Green Analytical Procedure Index (mogapi), Red Analytical Performance Index (RAPI), Red Green Blue Model (RGB) and Blue Applicability Grade Index (BAGI).

Methods: The Chromatographic separation was achieved using Inertsil ODS-3V (250 x 4.6 mm, 5 μ) column with the mobile phase of methanol: water (95:05) at the flow rate of 1 ml/min and run time was kept for 6 min and the wavelength for analysis was set at 260 nm.

Results: The Posaconazole was eluted from the column at 3.379 min and the proposed analytical method demonstrated that all the validation parameter was performed as per ICH Q2R1 recommendations and all the parameters are within the acceptable range. The calibration curve showed linear in the concentration range of 1 to 25 μ g/ml with a correlation coefficient of 0.9999.

Conclusion: The validated RP-HPLC method is accurate, precise, and reliable, showing superior performance, eco-friendliness, and high throughput compared to reported methods, as confirmed by green and white tools, making it suitable for systematic investigation of posaconazole in its formulation.

Keywords: AGREE, mogapi, RAPI, RGB, BAGI.



PA-QA-016

Determination of bispyribac-sodium, hexaconazole, quinalphos, and chlorpyrifos in fruits and vegetables by RP-HPLC method

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Background:

The main goal of this research is to develop a simple, sensitive, and fast method for determining the Methanol, Ethanol, 1-propanol, and 2-propanol in the raw materials used in the manufacturing of OTC products, as most of the methods applied require considerable time.

Aims & Objectives:

The research aims to quantify the pesticide residues of Bispyribac sodium, Hexaconazole, Quinalphos, and Chlorpyrifos, which are commonly used in agriculture to control pests in vegetables and fruits. This study also aims to provide a simple, effective, and repeatable HPLC method for quantifying four pesticide residues and their extraction method in vegetables and fruits. Validate the developed HPLC method as per ICH guidelines.

Methods: HPLC separation was performed using the gradient method of elution. The mobile phase was (A) acetonitrile: (B) 0.02% formic acid in water at a flowrate of 1.7 ml/min. The sample was injected into a volume of 10 µl. The column oven temperature remained at 430C throughout the chromatographic operation. The absorbance of these four pesticides was measured at an UV wavelength of 227nm using a PDA detector.

Results: The retention times for Bispyribac sodium, Hexaconazole, Quinalphos, and Chlorpyrifos were 4.162, 6.062, 9.043, and 13.980 minutes, respectively. The overall elution time was around 20 minutes.

Conclusion: The developed and validated RP-HPLC method is effective for the determination of bispyribac sodium, hexaconazole, quinalphos, and chlorpyrifos pesticides in vegetables and fruits. The methods were found to be accurate, precise, sensitive, robust, and easy to apply.

Keywords: RP-HPLC; pesticide residues; bispyribac-sodium; hexaconazole; quinalphos; chlorpyrifos; vegetables; fruits.



PA-QA-017

Simultaneous Analysis of Gefitinib and Berberine in Nano-Lipid Formulation for Breast Cancer Using aqbd Optimized UFLC Method

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Background:

The current research addresses the need for an efficient analytical method to simultaneously quantify Gefitinib (GEF) and Berberine (BER) in a nano-lipid carrier (NLC) formulation, developed as a combinational strategy for breast cancer treatment. Such dual-drug delivery systems require precise analytical control to ensure efficacy and quality.

Aims and Objective:

To develop and validate an Analytical Quality by Design (aqbd)-driven Ultra-Fast Liquid Chromatography (UFLC) method for the simultaneous estimation of GEF and BER in NLC formulations targeted for breast cancer therapy.

Methods:

The method was optimized using Box-Behnken Design, focusing on critical method parameters like acetonitrile: buffer ratio, buffer pH, and flow rate. Chromatographic separation was achieved on a C18 column with a mobile phase of acetonitrile: phosphate buffer (45:55, pH 5.1), at a flow rate of 1 ml/min, injection volume of 10 µl, and detection at 260 nm. Method validation followed ICH Q2 (R1) guidelines and included system suitability, linearity (1–20 µg/ml), accuracy, precision, specificity, robustness, LOD, and LOQ. Forced degradation studies under acidic, basic, oxidative, and thermal conditions were also performed.

Results:

The method demonstrated excellent system suitability and peak resolution. Linearity was observed with $R^2 > 0.990$. Accuracy ranged between 98–102% recovery, and precision showed %RSD below 2%. LOD and LOQ were 0.065 µg/ml and 0.16 µg/ml for GEF, and 0.022 µg/ml and 0.20 µg/ml for BER. Entrapment efficiencies were 81.8% for GEF and 89.6% for BER. The nlc's showed favourable particle size and polydispersity index, supporting their applicability for targeted delivery.

Conclusion:

The validated aqbd-driven UFLC method is robust, precise, and suitable for routine quality control of dual-drug NLC formulations. It supports the analytical needs of combinational drug delivery strategies in oncology, particularly for breast cancer treatment.

Keywords:

Gefitinib, Berberine, Nano Lipid Carrier, UFLC, aqbd, Breast Cancer, Method Validation



PA-QA-018

Development and Validation of a High-Performance Thin-Layer Chromatography (HPTLC) method for quantitative estimation of Sotagliflozin in bulk drug form.

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Background:

Sotagliflozin, which is marketed under the brand name Inpefa, was approved by the USFDA for the treatment of heart failure on May 26, 2023. Existing literature reports its estimation using UPLC with a photodiode array detector but no HPTLC method has been reported for its quantification. Hence, the present study aimed to develop and validate a simple, specific, and reliable HPTLC method for the determination of Sotagliflozin in bulk drug form. The method was validated according to the ICH guidelines Q2(R2).

Aims & Objectives:

Aim

- To develop and validate a HPTLC method for estimation of Sotagliflozin.

Objectives

- To develop a precise, repeatable and accurate HPTLC approach for evaluation of Sotagliflozin.
- To validate the developed method according to ICH guidelines Q2(R2) for intended analytical application.

Methods:

The HPTLC method was developed using a CAMAG Linomat 5 sample applicator equipped with a UV detector. Samples were applied in the form of 6 mm wide bands using a CAMAG microliter syringe on precoated silica gel G60 F254 aluminum plates (Merck, Germany).

Results:

Linearity - correlation coefficient (r^2) was found to be 0.9994

Accuracy – 99.00% to 99.75%

Precision – 0.06

LOD & LOQ (ng/band) – 0.48 & 1.47

Ruggedness – 0.06

Robustness - %RSD $\leq$ 2%

Conclusion:

This study presents a simple, validated HPTLC method for the estimation of Sotagliflozin. The developed method is sensitive, specific, rapid, robust, precise, and accurate. The validation results confirm that the method complies with the ICH Q2(R2) guidelines. Therefore, it can be concluded that this method is suitable for the routine analysis of Sotagliflozin in bulk form using HPTLC.

Keywords:

Sotagliflozin, HPTLC, Method development, Method validation, SGLT2 inhibitor.



PA-QA-019

Development and validation of stability indicating method for Udenafil in bulk by HPLC

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Background:

Forced degradation studies typically involve the exposure of representative sample of the drug substance or drug product to the relevant stress conditions of light, heat, humidity, acid/base hydrolysis and oxidation. The performance characteristics of assay validation include specificity, accuracy, precision, limit of detection, limit of quantitation, linearity, range, and robustness.

Aims & Objectives:

To Develop and Optimize HPLC Chromatographic Conditions for Udenafil. To develop the stability-indicating analytical method for Udenafil using forced degradation studies. To validate the developed method using ICH Guidelines.

Methods:

Method Development - Selected reverse phase HPLC for drug separation due to its specificity and sensitivity. Optimized chromatographic parameters: detection wavelength, stationary phase, and mobile phase ratio. Optimized HPLC Chromatographic conditions were used. Performance of forced degradation studies such as Acid degradation, Base/Alkali degradation, Neutral degradation, Oxidative degradation and Photolytic degradation. Analytical method validation parameters Linearity and range, Limit of Detection (LOD), Limit of Quantification (LOQ).

Results:

Optimization of HPLC Conditions Selection of UV detection wavelength at 291 nm for Udenafil was established based on spectral analysis (200-400 nm). The initial mobile phase included Acetonitrile and Methanol for effective drug elution. Use of Sodium dihydrogen orthophosphate dihydrate (ph 6.0) resulted in improved peak asymmetry and resolution. Forced degradation studies, such as Acidic conditions resulted in 36.9% degradation after 24 hours; Basic condition 23.5% degradation after 24 hours; Neutral Condition 28.8% degradation after 24 hours; Oxidative Condition 25.8% degradation after 24 hours; and Photolytic Condition 26.8% degradation after 24 hours. The linearity range was 1-20 ($\mu\text{g/ml}$). LOD was found to be 0.7621, and LOQ was found to be 2.3095.

Conclusion:

The current approach was developed and validated utilizing parameters such as accuracy, precision, linearity, and system applicability. The acquired data was determined to be more sensitive and was well within the prescribed limits.

Keywords:

Udenafil, method development, forced degradation studies,



PA-QA-020

An optimization of Analytical and Bioanalytical methods for Estimation of Anti-viral Drug in Pharmaceutical Formulation

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Background: In order to estimate the Sofosbuvir in its marketed formulation and biological fluid we have few analytical methods. The reported UV and HPLC methods for the Sofosbuvir involves the costlier, less sensitive and tedious mobile phase usage. So, there is need for development of simple, sensitive and economical analytical method for the determination of Sofosbuvir. To overcome the limitations associated with the reported methods there is a need to develop and validate new bioanalytical and analytical method for the estimation of selected Sofosbuvir as per current regulatory requirements.

Aims & Objectives: The aim and objectives are to develop and validate novel analytical and bioanalytical method to quantify selected anti-viral drug in its marketed formulation and biological fluid as per regulatory guidelines.

Methods: The UV method and HPLC method were developed. The developed methods were validated as per ICH guidelines such as specificity, selectivity, linearity, precision, robustness, ruggedness and accuracy. Newly developed and validated methods were successfully applied for standardization of antiviral drug in pharmaceutical formulation.

Results: An anti-viral drug exhibits λ_{max} at 260nm and concentration range of 10 to 50 $\mu\text{g/ml}$ for both UV and HPLC obeys the beer's law. LOD was found to be 1.20 $\mu\text{g/ml}$ for UV and 2.19 $\mu\text{g/ml}$ for HPLC. The LOQ was found to be 1.899 $\mu\text{g/ml}$ for UV and 6.63 $\mu\text{g/ml}$ for HPLC. Accuracy of drug in pharmaceutical formulation was observed in the range of 90-110%. All the repeatability and precision results were within acceptable range i.e. Less than 2%.

Conclusion: Both the methods were found to be precise, simple, accurate, reproducible and can be used for routine estimation analysis of Sofosbuvir in bulk and pharmaceutical formulation.

Keywords: Anti-viral drug, Bioanalytical method, Quantification, Standardization



PA-QA-021

Formulation and Characterization of Liquid Crystalline Nanoparticles for Cyclosporine Delivery: Entrapment, Release Profile, and Analytical assessment

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Background:

Cyclosporine (csa), a widely used oral immunosuppressant with antifungal properties, suffers from extremely low aqueous solubility due to its highly lipophilic cyclic undecapeptide structure, leading to poor membrane permeability. Formulating csa into liquid crystalline nanoparticles (lcns) can significantly enhance its solubility and bioavailability. However, no validated analytical method has been specifically reported for csa estimation in such LCN formulations.

Aim & Objectives:

To design and validate a rapid, a dependable reverse-phase high-performance liquid chromatographic (RP-HPLC) approach with a UV detector for quantitative determination of csa in lcns. This method is also applied to evaluate drug loading (DL%), drug entrapment efficiency (DEE%), and to analyze in vitro drug release samples.

Methods:

Using a Shim-pack GIST C18 column (4.6×100 mm, $5 \mu\text{m}$) and a mobile phase made up of acetonitrile and 10 millimolar ammonium acetate buffer (ph of 4.0) with a 90:10 ratio, the separation by chromatography was achieved. A $20 \mu\text{l}$ injection volume, a column temperature of 50°C , a detection wavelength of 215 nm , and a flow rate of 0.8 ml/min have been maintained.

Results:

The developed RP-HPLC method demonstrated great accuracy, precision, and reproducibility after being validated in accordance with ICH requirements. With LOD and LOQ values of $0.12 \mu\text{g/ml}$ and $0.15 \mu\text{g/ml}$, respectively, the technique showed great sensitivity and excellent linearity over the $1\text{--}64 \mu\text{g/ml}$ range. The accuracy, precision, and durability of the approach for accurate analyte quantification were further validated by consistent recovery values ranging from 98% to 100%. With a run time of about ten minutes, csa peak appeared at 4.56 mins. For precision studies, the %RSD maintained below 2%. Csa-liquid crystal nanoparticles demonstrated 83.13% entrapment efficiency and $5.90 \pm 0.31\%$ drug loading. The release profile demonstrated a controlled, sustained drug release compared to free csa.

Conclusion:

The validated RP-HPLC approach offers a robust, sensitive, and efficient technique for csa quantification in liquid crystalline nanoparticles, enabling accurate assessment of DL%, DEE%, and release kinetics.

Keywords:

Cyclosporine (csa), liquid crystalline nanoparticles (lcns), RP-HPLC, method validation, drug loading, entrapment efficiency, sustained release.



PA-QA-022

Targeted drug delivery approaches for the treatment of *Helicobacter pylori* infection

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Helicobacter pylori (H. Pylori) is a gram-negative, rod-shaped bacterium that infects half of the world population. It is generally transmitted through the oral-oral, fecal-oral route, and an untreated infection may lead to peptic ulcer disease and gastric cancer. Due to high antibiotic resistance and poor patient compliance, current treatment regimens face significant challenges. This demands the development of novel, targeted strategies for eradicating H. Pylori. The developing field of targeted nanotherapeutics presents an effective alternative. It involves conjugating the ligands to the nanoparticles for targeting various receptors present on the bacteria. This not only enhances local drug concentration near the H. Pylori but also exhibits other activities such as inhibiting adhesion to the gastric mucosa, damaging the bacterial cell wall, minimal impact on gut microbiota, etc. These nanotherapeutics have shown promising results, improving bacterial eradication, minimal damage to the gut microbiota, and decreasing drug resistance. Despite ongoing difficulties in clinical translation, targeted nanotherapeutics provide a critical pathway to overcome current treatment challenges and to improve treatment outcomes for H. Pylori infection.



PA-QA-023

Recent Advancements and Developments in Investigation of Peptide Aggregation for Alzheimer's Disease Using AIML- Variational Autoencoders, doe Software, and Spectroscopic Detection Techniques

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Introduction: Alzheimer's Disease is responsible for the gradual decline of cognitive function, thinking, language & problem-solving ability, associated with the accumulation of Amyloid-Beta ($A\beta$) plaque and neuro-fibrillary tangles, composed of tau-protein in the brain, which disrupts neuronal signaling, & causes neuronal loss. Thus, understanding and mitigation of $A\beta$ -aggregation is crucial. Addressing $A\beta$ -aggregation requires innovative approaches that combine advanced technologies.

Methodology: This study focuses on AIML models including Deep Generative Models (dgms)- Variational Autoencoders (vae), for predicting design of possible new peptides and aggregation-resisting peptides by prediction of Aggregation-Prone Regions (aprs) & designing novel peptides resistant to misfolding. By Principles of Design of Experiment (doe), process parameters to generate best suitable combinations & factor selection- for formulation protocol inputs to ensure robust & scalable design is optimized. Multiple factors influence aggregation, Thus, need for real-world verification of designs prepared from AI-doe tools is done by Spectroscopic techniques, Including UV-Vis, Fluorescence and CD Spectroscopic methods in analysis of β -sheet formation (2° structural changes), Conformational transitions, Impurity Profiling, and understanding self-assembling behavior. This Combination bridges the gap between computational predictions & real-world validation.

Results: The study successfully demonstrated synergistic efficacy of AI tools with Spectroscopic analysis in understanding & mitigation of $A\beta$ -aggregation. By Craftmanship of doe & dgms, structural change at specific regions were predicted & novel therapeutic peptides were designed. Overall, it provided significant strides in peptide therapies for Alzheimer's.

Conclusion: This multidisciplinary approach offers a comprehensive solution to address $A\beta$ -aggregation. Additionally, these advancements hold promise for expanding applications to other neurodegenerative diseases.

Keywords: Alzheimer-Targeted Peptide Design, Amyloid- β Aggregation, AI-Driven Generative Models, doe for Optimization, Advanced Spectroscopic Analysis.



PA-QA-024

Development And Validation of an Analytical Method for Simultaneous Estimation of Atenolol and Hesperidin: An Interaction Study

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Aim:

To develop a validated analytical method for simultaneous estimation of Atenolol and Hesperidin as per ICH guidelines.

Methods:

The chromatographic separation was achieved by using (Accucore C₁₈, 50mm x 4.6, 5μ particle size) column by applying gradient elution using the mobile phase A consist of in water as an aqueous phase and the following gradient in the ratio initial (95% A and 5%) buffer is maintained for 0 to 1.4 minutes ,and then from 1.5 to 5.9 minutes (95%A and 5%B) and from 6 to 6.9 minutes(5%A and 95%B) and then from 7 to 7.9 minutes (95%A and 5%B) and in 8 minutes (95%A and 5%B) was maintained. 95:5 (v/v) detection was carried at the 230 nm by employing 0.5 ml/min flow rate.

Results:

The retention time was found to be 3.00 min and 3.97 min for Atenolol and Hesperidin respectively. The developed method has the linearity range was obtained for HPLC method was 100 μg/ml and 50μg/ml for Atenolol and Hesperidin respectively and the regression coefficient (r^2) is 1.00 and 0.995 for the both drugs. Accuracy and precision are evaluated for the method and found be within the limits and the results were reproducible.

Conclusion:

Based on these results, conclude that the developed method was precise and accurate for the simultaneous estimation of Atenolol and Hesperidin. This method can be adopted for simultaneous estimation of drugs and will be helpful for in-vivo studies in future days & pharmacokinetics studies.

Keywords: Atenolol, Hesperidin, Validation, High Performance Liquid Chromatography,



PA-QA-025

RP-HPLC Method for the Estimation of Mangiferin in Nano Formulations: Development and Optimization by Analytical Quality-by-Design

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Background: Mangiferin (MGF), a naturally occurring polyphenol, possesses a wide range of pharmacological properties, including neuroprotective effects. However, its clinical application is hindered by low solubility and bioavailability. Lipid-based nanoformulations like Solid-Lipid Nanoparticles (SLNs) can overcome these limitations, but their development requires a sensitive and robust analytical method for accurate drug quantification, which is currently lacking.

Aims & Objectives: The primary objective of this study was to develop, optimize, and validate a simple, robust, and sensitive reverse-phase high-performance liquid chromatography (RP-HPLC) method for the estimation of MGF in nanoformulations by employing an Analytical Quality-by-Design (AQbD) approach.

Methods: The AQbD framework was utilized for systematic method development. Critical Method Parameters (CMPs) were screened using a Taguchi Orthogonal Array design, followed by optimization using a Box-Behnken Design (BBD). Chromatographic separation was achieved on a Hyperclone C18 column using an isocratic mobile phase of phosphate buffer (pH 3.2) and a mixture of acetonitrile and methanol (30:70) in a 78:22% v/v ratio, at a flow rate of 1.0 mL/min. Detection was performed at 258 nm. The method was validated according to ICH Q2(R1) guidelines.

Results: The optimized method demonstrated excellent linearity over a concentration range of 50-5000 ng/mL with a correlation coefficient (R^2) of 0.9999. The method was found to be highly sensitive, with a limit of detection (LOD) of 1.43 ng/mL and a limit of quantitation (LOQ) of 4.36 ng/mL. Validation studies confirmed the method's accuracy, precision, and robustness, with %RSD values well within acceptable limits. The method was successfully applied to determine the drug content of MGF-loaded SLNs and to evaluate in-vitro drug release kinetics.

Conclusion: A scientifically sound, robust, and sensitive AQbD-driven RP-HPLC method was successfully developed and validated for the quantification of MGF. The method is cost-efficient, requires minimal organic solvent, and is suitable for routine quality control and stability testing of MGF in both bulk and nanoformulation systems.

Keywords: Analytical quality by design (AQbD), RP-HPLC, Mangiferin, Nanoformulation

Category 4

Pharmacognosy and Phytomedicine



PCO-PM-001: Fabrication and Characterization of Sodium Alginate Wound Dressing Containing *Tridax procumbens* Linn Leaf Extract

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Background:

- Dermal wound is a common pathologic condition and may be defined as any break in the integrity of the skin.
- Skin wounds have a tremendous negative impact on healthcare systems and the economy worldwide.
- It was reported recently that nearly one billion people suffer from acute and chronic wounds globally.

Aims & Objectives:

Aim

To fabricate and characterize the sodium alginate wound dressing containing *Tridax procumbens* aqueous leaf extract for treating wounds.

Objectives

1. To collect and authenticate the *T. Procumbens* leaves.
2. To prepare the aqueous extract of *T. Procumbens* leaves.
3. To perform the phytochemical constituents of prepared extract.
4. To evaluate the antibacterial and antioxidant potential of the extract.
5. To fabricate Sodium alginate wound dressing containing the prepared extract.
6. To study physiochemical characterization of the fabricated wound dressing such as swelling index, SEM analysis, folding endurance, tensile strength, etc.

Methods:

- **Collection and Authentication:** Leaves of *Tridax procumbens* Linn were collected locally and authenticated at the Botanical Survey of India, TNAU Campus, Coimbatore.
- **Preparation of Aqueous Extract:** Dried leaf powder was added to boiling water, filtered after 30 minutes (Whatman paper), and concentrated using a water bath. The residue (TAE) was stored in a desiccator.
- **Phytochemical Evaluation:** TAE was subjected to standard chemical tests for steroids, tannins, saponins, alkaloids, flavonoids, phenols, proteins, and diterpenes.
- **Pharmacological Screening:** Antioxidant activity was assessed by mixing 100 μ l of 0.01% DPPH in methanol with 100 μ l of extract at various concentrations in a 96-well plate. After 30 minutes in the dark, absorbance was measured at 517 nm (BIO-RAD). Methanol served as the control.

Results: The aqueous extract of *Tridax procumbens* leaves (TAE) yielded 26.7% w/w, appearing as a brown powder. Phytochemical screening confirmed the presence of tannins, saponins, alkaloids, phenols, proteins, amino acids, and diterpenes. HPTLC analysis identified the presence of rutin and kaempferol, supporting earlier reports. Although TAE showed no significant antibacterial activity compared to ciprofloxacin, it demonstrated dose-dependent antioxidant activity with an IC₅₀ of 81.14 μ g/ml (ascorbic acid: 14.2 μ g/ml). MTT assay on HEK 293 cells indicated >95% cell viability, suggesting its safety and potential for wound healing. Swelling index studies revealed that higher calcium chloride concentration reduced swelling but increased folding endurance, with formulation F5 (0.3% TAE) showing optimal properties. FTIR analysis confirmed molecular interaction between TAE and sodium alginate



without altering major functional groups. SEM images of TAE films showed uniform, crack-free surfaces with increased roughness. The tensile strength of the film decreased slightly with TAE addition (83 mpa to 72 mpa) but remained mechanically stable.

Conclusion:

- This comprehensive study highlights the potential of *Tridax procumbens* aqueous extract (TAE) in wound healing, displaying diverse phytochemicals, favourable antioxidant effects and cell proliferation.
- The overall study concludes the developed sodium alginate wound dressing incorporated with TAE having potential applications in dermal wound healing.

Keywords: Tridax procumbens, wound healing, aqueous extract, film, sodium alginate



PCO-PM-002: Preclinical evaluation of wound healing properties of novel ayurvedic formulations

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Background: Wound healing is a complex biological process involving haemostasis, inflammation, proliferation, and remodelling. Despite advances in conventional treatments, chronic and non-healing wounds remain a clinical challenge. Recent clinical observations have highlighted the therapeutic benefits of a novel Ayurvedic formulations, comprising a polyherbal oral syrup and a topical oil, in managing chronic wounds of various aetiologies. However, experimental validation of these effects in controlled settings has been limited. The present study focuses on evaluating the wound healing efficacy of these formulations in a full-thickness excision wound model in healthy Wistar rats, to preliminarily assess their healing potential and histological impact under normal conditions.

Methods: After the ethical committee clearance, under anaesthesia, excision wounds (2 cm in diameter and 0.2 cm depth) were surgically created on the dorsal surface of normal 10-12 months old Wistar rats. The animals were randomized into four groups (n=5): Group I – Control, Group II – Standard (recombinant human epidermal growth factor gel, topical), Group III – Formula 1 (oral syrup), and Group IV – Formula 1 + 2 (oral syrup + topical oil). Wound closure was monitored on alternate days through photographic documentation and wound tracing. The percentage of wound contraction was calculated using imagej software. Skin samples were harvested on days 8 and 16 for histopathological evaluation using haematoxylin-eosin and Masson's trichrome staining.

Results: Healing was rapid in all treated groups in comparison to control group. However, the group treated with the combination of Formula 1 + 2 exhibited the most significant wound closure and histological improvements, including enhanced epithelialization and granulation tissue formation indicating the synergistic effect of oral and topical formulations.

Conclusion: The findings from this preliminary study demonstrate that the novel Ayurvedic formulation, particularly when administered in combination as oral syrup and topical oil, significantly enhances wound healing in normal rats compared to untreated and standard groups. These results provide initial preclinical evidence supporting the efficacy of this Ayurvedic formulations as a promising alternative therapy for promoting cutaneous wound healing under normal physiological conditions and may be useful in treating non-healing types of wounds in different medical conditions.



PCO-PM-003: Formulation and Evaluation of an Anti-Bacterial Herbal Face Pack: A Comparative Study of Orange Peel and Lychee Peel Extracts

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Background: Skin issues like acne, pimples, and infections are often caused by bacteria, pollution, and excess oil. While synthetic products offer fast results, they can cause side effects with long term use. Herbal face packs provide a safer, natural alternative with benefits like cleansing, exfoliation, and antibacterial action. This project aims to formulate and evaluate an antibacterial herbal face pack using ingredients such as Multani mitti, neem, turmeric, gram flour, cucumber, aloe vera, rose petals, and rosemary, all known for their skin protective properties. A comparative study was conducted using orange peel and lychee peel, both rich in antioxidants and antibacterial compounds, to assess which offers better efficacy. The formulations were evaluated for physical and chemical properties, and antibacterial activity was tested against *Staphylococcus aureus* using the agar well diffusion method. This study supports the use of natural ingredients for effective and safe skincare.

Aims & Objectives: To evaluate the antibacterial potential of herbal face packs formulated using orange peel and lychee peel, with comparative analysis based on physicochemical, microbiological, and safety assessments

Methods: Herbal face packs were formulated using natural ingredients, with orange peel and lychee peel as the key components. Two formulations were prepared one with orange peel and the other with lychee peel along with common herbal bases (Multani mitti, neem, turmeric, etc.). Physicochemical parameters such as pH, texture, and spreadability were evaluated. Antibacterial activity was assessed against *Staphylococcus aureus* using the agar well diffusion method. Zones of inhibition were measured to compare the efficacy of both formulations. Safety evaluation included skin irritancy and washability tests conducted on human volunteers under ethical approval.

Results: The F2 formulation (lychee peel-based) demonstrated improved physicochemical characteristics and superior antibacterial activity compared to F1 (orange peel based). Both formulations showed acceptable pH for skin application, were easily washable, and caused no irritation. Antibacterial assays revealed that F2 had a larger zone of inhibition against *Staphylococcus aureus*, indicating better antimicrobial potential. Overall, F2 exhibited more favorable properties for use as a cosmetic herbal face pack.

Conclusion: The formulated herbal face pack containing **lychee peel** (Formulation 2) demonstrated superior antibacterial activity compared to the **orange peel formulation** (Formulation 1), along with acceptable physicochemical characteristics and no observed skin irritation. These findings support the potential of **lychee peel** as an effective natural antibacterial agent for cosmetic applications. Further studies can evaluate its long term stability, broader antimicrobial spectrum, and consumer acceptability.

Keywords: Herbal face pack, Orange peel, Lychee peel, Antibacterial activity, Natural cosmetics, Skin irritation test, Physicochemical evaluation, Multani mitti, Neem, Aloe vera



PCO-PM-004: Formulation and evaluation of non-fluoridated polyherbal toothpaste

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Background: Oral health is extremely important for general well-being. Traditional toothpastes that use chemicals like fluoride and sodium lauryl sulfate (SLS) have demonstrated undesirable side effects including mucosal irritation, cytotoxicity, and ulcers. Over the past few years, herbal products have proven to be safer alternatives because of their antimicrobial, antioxidant, and anti-inflammatory activities

Aims & Objectives:

- To develop a non-fluoridated polyherbal toothpaste from the extracts of Parijat leaves (*Nyctanthes arbor-tristis*), Areca husk (*Areca catechu*), and Mango leaves (*Mangifera indica*).
- To study the physicochemical characteristics and antimicrobial activity of the developed toothpaste.
- To assess the antibacterial activity against a standard drug (Clindamycin IP).

Methods:

Herbal extracts were collected through alcoholic maceration and analyzed for phytochemical constituents. Toothpaste samples were formulated utilizing ingredients such as cocoglucoside, glycerin, methylcellulose, and calcium carbonate. The samples were tested through physical tests such as pH, foamability, homogeneity, moisture content, shape retention, spreadability, and ash value. Antibacterial activity was determined through agar well diffusion against *Staphylococcus aureus* (Gram-positive) and *Escherichia coli* (Gram-negative).

Results: The extracts showed the presence of alkaloids, flavonoids, tannins, and saponins. The pH levels in the formulations varied from 7.2–7.5, foamability varied from 14–25 ml, and moisture level varied from 16–20.2%. Antibacterial activity indicated that formulation F3 showed the largest zone of inhibition: 2.7 cm for *S. Aureus* and 2.4 cm for *E. Coli*, similar to the standard drug.

Conclusion: The synthesized polyherbal toothpaste exhibited excellent antibacterial activity and good physicochemical properties. It is a safe and efficient alternative to market-available fluoridated toothpastes and advocates the utilization of medicinal plant extracts in dental care products.

Keywords: Polyherbal toothpaste, *Areca catechu*, *Mangifera indica*, antibacterial activity, non-fluoridated toothpaste, herbal oral care, phytochemical screening



PCO-PM-005: Modulation of Monoaminergic and Inflammatory Pathways by LC-MS Identified Phytocomponents of *Cynodon dactylon* in a Chronic Unpredictable Stress Model of Comorbid Depression

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Background: Depression is a major psychiatric disorder often coexisting with neuropsychiatric conditions like anxiety. Factors such as prolonged working hours, disturbed sleep cycles, and increasing mental stress in modern lifestyles contribute to elevated levels of psychological distress, leading to anxiety and depression

Aim: To evaluate the therapeutic potential of *Cynodon dactylon* extract in comorbid depression using a chronic unpredictable stress (CUS) model in rats.

Objectives:

- To identify the phytochemical constituents of *C. Dactylon* extract through LC-MS analysis.
- To assess the impact of the herbal extract on neuronal count, neurotransmitter levels, and inflammatory markers in the hippocampus, compared to a standard antidepressant.

Methods: The hydro-alcoholic extract of *C. Dactylon* was subjected to LC-MS analysis to find the active component. Wistar rats were exposed to CUS to induce comorbid depression. Rats in the treatment group received *C. Dactylon* extract orally at 400 mg/kg body weight. Post-treatment, hippocampal tissues were analysed for histological analysis of neuronal count. Neurotransmitter (norepinephrine, serotonin, dopamine, GABA) levels and inflammatory markers (IL-6, homocysteine) were quantified using ELISA kits.

Results: LC-MS analysis revealed harmine as a major component, along with ergosterol, colchicine, syrotingopine, and propyl gallate. The stress group exhibited significantly reduced monoamine neurotransmitters and GABA levels, and elevated IL-6 and homocysteine levels. Treatment with *C. Dactylon* significantly reversed these changes ($P < 0.001$), with results showing a marked increase in neurotransmitter levels and a decrease in inflammatory markers when compared to both stress and antidepressant-treated groups. The extract-treated group also showed a significantly higher neuronal count in hippocampus indicating enhanced neuroprotection.

Conclusion: These findings suggest that *C. Dactylon* holds promising therapeutic potential as a natural intervention for managing depression and its associated neuroinflammatory changes.

Keywords: Depression, anxiety, stress, herbal extract, neurotransmitters, inflammatory markers.



PCO-PM-006: Comparative Role of *Allium* Extracts Versus Conventional Therapy on Neurodegenerative and Neurobehavioral Markers in a 6-OHDA-Induced Rat Model of Parkinson's Disease

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Background: Parkinson's disease (PD) is a progressive neurodegenerative disorder characterized by damage to dopaminergic projections leading to motor dysfunction, cognition and behavioural variations. A key pathological hallmark is the abnormal aggregation of alpha-synuclein into Lewy bodies. Reduced levels of progranulin (PGRN) are associated with accelerated neurodegeneration, while decreased brain-derived neurotrophic factor (BDNF) impairs learning, memory, and motor coordination. *Allium* vegetables represent a promising intersection of nutrition and neuropharmacology,

Aims & Objectives: To evaluate the neuroprotective effects of *Allium sativum* and *Allium cepa* extracts versus conventional therapy on neurodegenerative biomarkers alpha-synuclein, PGRN, and BDNF and their correlation with cognitive, behavioral, and motor functions in Wistar rat model of PD.

Methods: All procedures were adhered to animal ethical guidelines. *Allium sativum* and *Allium cepa* extract powders were sourced from a certified pharmaceutical company. LC-MS analysis was conducted at Dextrose Pvt. Ltd. Wistar rats (150–220 g) were randomly assigned to Control, Sham-Lesioned, Lesioned, and Treatment groups. Parkinsonism was induced via intrastriatal injection of 6-hydroxydopamine (6-OHDA) using a stereotaxic apparatus. Treatment groups received *Allium sativum*, *Allium cepa*, and levodopa + carbidopa for 50 days. Cognition, behavioural variations and sensorimotor coordination were assessed. On day 50, rats were euthanized, and brain regions (cortex, striatum, hippocampus) were analysed for alpha-synuclein, BDNF, and PGRN in neuronal assays.

Results: Both *Allium* extracts significantly improved motor coordination and reduced anxiety-like behavior compared to the 6-OHDA group. Treatment with *Allium* extracts and conventional therapy reduced alpha-synuclein levels while increasing BDNF and PGRN expression. Behavioral recovery and biomarker regulation were most pronounced in combination therapy groups.

Conclusion: *Allium* extracts, individually or combinational therapy, demonstrate promising neuroprotective potential by enhancing neurotrophic support, and reducing neurodegenerative markers. Further research into their mechanistic role could advance therapeutic strategies highlighting their value as a nutritional phyto-medicine.

Keywords: Parkinson's disease, *Allium sativum*, *Allium cepa*, alpha-synuclein, BDNF, progranulin,



PCO-PM-007: Exploring the Therapeutic Spectrum of *Dichrostachys cinerea* (L.) Wight & Arn. Extracts in Rheumatoid Arthritis: An Integrative Preclinical and Docking Study
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The leaves of *Dichrostachys cinerea* (L.) Wight & Arn. (Fabaceae) have traditionally been used to treat arthritis. Therefore, this study aimed to evaluate the anti-arthritic potential of the alcoholic (DCA) and aqueous (DCW) extracts of *Dichrostachys cinerea* (*D. Cinerea*) using the Freund's complete adjuvant (FCA) model. *D. cinerea* was extracted using alcohol via the Soxhlet method and water through the reflux method. The resulting alcoholic (DCA) and aqueous (DCW) extracts were screening for the presence of the phytochemicals by chemical test and TLC analysis. A combination of network pharmacology and molecular docking was used to predict key targets and evaluate the binding interactions of selected phytochemicals, providing a mechanistic understanding of their potential therapeutic roles. Their anti-arthritic potential was evaluated in female Wistar rats using the Freund's Complete Adjuvant (FCA)-induced arthritis model, with methotrexate serving as a positive control. Parameters such as paw volume, arthritic score, ALP, ALT, serum urea, CRP, RF levels, histopathological examination of liver tissues, and radiological assessments were analyzed to characterize the activity of the DCA and DCW extracts.

Network pharmacology identified the PI3K/AKT pathway as a key target of selected phytoconstituents. Molecular docking showed strong binding of quercetin-3-O-glucoside to PI3K/AKT, suggesting its potential to modulate cancer-related signaling. The DCA and DCW extracts, administered at a dose of 350 mg/kg b.w. (p.o.), along with methotrexate, significantly inhibited paw volume ($p \leq 0.03$) and reduced the arthritic score. In contrast to the disease control group, the DCA-treated animals exhibited a notable reduction in ALP, ALT, serum urea, CRP, and RF levels. Histopathological analysis revealed a decrease in inflammatory cell infiltration, while the radiological assay indicated reduced degenerative changes in joint following DCA treatment.

This study validates the traditional use of *Dichrostachys cinerea* by scientifically proven by pre-clinical studies that the DCA extract exhibits stronger anti-rheumatoid arthritis activity than the DCW extract.

Keywords: Arthritis, Methotrexate, Flavonoids, Inflammation, Radiological assay.

PCO-PM-008: Potential role of ashwagandha [withania somnifera] as an antioxidant on aluminium induced brain tissue damage in wistar rats

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Background: Aluminium is most prevalent and third most abundant element in earth's crust after oxygen. Its exposure in high concentration can accumulate in many organs that damages various organs in living organisms like humans and animals. Although aluminium (Al) is known to induce oxidative damage through various mechanisms including binding to negatively charged phospholipids on the membrane of various tissue cell which are rich in PUFA.

Aim & Objectives: This study was aimed to find the potential role of ashwagandha on aluminium induced brain toxicity.

Methods: Animals were segregated into 4 groups of 6 rats in each. The control group, the Ashwagandha treated group, the Aluminium intoxicated group, pretreated with Ashwagandha for Aluminium toxicity group. Brain tissue was removed and were stored in 10% formalin saline and histopathological slides were done. A part of the tissues were processed for estimation of MDA and GSH level.

Results: In the present study administration of aluminium in rats showed a significant decrease in the tissue level of GS and increase in the level of MDA in aluminium treated group compared to normal control. Treatment with Ashwagandha showed a significant increase in GSH level and decrease in MDA level. Photomicrographic sections of the Brain in Ashwagandha-treated rats showed a Normal Neuronal Count. But, exposure to Aluminium has caused significant reduction in neuronal count. Neuronal count in the experiment group pretreated with ashwagandha showed a visible increase in neuronal count in different regions of the Hippocampus, Dentate Gyrus and Frontal Cortex of rat brain when compared to Aluminum intoxicated group.

Conclusion: The results of this study revealed that oral aluminium administration induced adverse oxidative effects on the exposed animals and treatment with *W. Somnifera* reduced the extent of aluminium chloride-induced tissue injury

Keywords: *Withania Somnifera*, Aluminum Chloride, Reactive Oxygen Species, Reduced glutathione, Malondialdehyde.

PCO-PM-009: Diosgenin for the Management of Osteoarthritis: Challenges in Therapeutic Delivery and Strategies to Overcome Them

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Background: Osteoarthritis (OA) is a chronic inflammatory joint disease characterized by cartilage destruction and pain. Although present therapies provide symptomatic benefit, they can be accompanied by side effects and restricted disease-modifying action. Diosgenin, a steroidal saponin of Dioscorea origin, has been shown to possess anti-inflammatory and cartilage-conserving activities and thus can be a promising candidate for the treatment of OA.

Aims & Objectives: To assess the pharmacological potential of Diosgenin in the treatment of OA, determine key issues in its clinical utility, and discuss innovative delivery systems to improve its therapeutic effectiveness.

Methods: A comprehensive review of preclinical and formulation-related studies on Diosgenin's anti-osteoarthritic activity was conducted. The essential pharmacokinetic drawbacks and delivery methods, such as nanogels and transdermal carriers, were thoroughly examined.

Results: Diosgenin downregulates the pro-inflammatory mediators TNF-alpha, IL-1beta, and COX-2 and promotes the survival of chondrocytes. Its low water solubility, poor bioavailability, and fast metabolism limit its effectiveness. Nano-based delivery systems such as transthesosomal nanogels have been found to possess improved skin penetration, controlled release, and targeted delivery to the diseased joints, offering substantial improvement in therapeutic efficacy.

Conclusion: Diosgenin has the potential to be a phytoconstituent for the management of osteoarthritis. Poor solubility and bioavailability problems associated with formulation can easily be overcome with newer drug delivery systems, particularly lipid-based nanocarriers.

Keywords: Diosgenin, Osteoarthritis, Phytoconstituent, Anti-inflammatory, Nanogels, Drug Delivery



PCO-PM-010: Synergistic effect of *Carica papaya* and *Muntingia calabura* in anti-breast cancer activity (MCF7): Evidences from in vitro and in silico studies

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Introduction: Breast cancer is the most prevalent type of cancer that affects women globally. The aim of this study is to evaluate the synergistic effect of *Muntingia calabura* and *Carica papaya* in the treatment of breast cancer using MCF 7 cell lines.

Materials and Methods: MCCP leaf extract were prepared using Soxhlet apparatus method, then separate extracts were combined in equal proportions further, the extract were investigated for the presence of phytoconstituents and TLC. Using MTT Assay, the anticancer activity of the MCF 7 cells was assessed. Further, LCMS had done to determine the potential bioactive components responsible for the anticancer activity, Following LCMS docking studies were performed with the help of receptors $\text{er}\alpha$, $\text{er}\beta$ & Progesterone to identify the optimal interaction.

Results: The Phytochemical profile reveals the presence of major phytoconstituents. TLC provides qualitative determination of the possible number of components. MTT showed that at the concentration of 100 $\mu\text{g/ml}$ significant anticancer activity had been produced. LCMS allowed determination of the major bioactive components. Docking studies were performed for six major compounds namely Uracil, Styrene, Formononetin, Myricetin, Safingol, Apocynin against three receptors Estrogen α , β , & Progesterone among those Formononetin & Myricetin showed strongest interaction.

Conclusions: The present work clearly shows the synergistic potential of MCCP leaf extract in the treatment of Breast cancer employing MCF-7 cell line model and also our studies contribute fresh insights into the potential of natural medicine as a viable & effective alternative. Hence natural remedies hold great promise in the realm of healthcare and cancer therapy.

Keywords: *Carica papaya*; *Muntingia calabura*; MCF 7; MTT assay; Estrogen receptors; Progesterone receptors;



PCO-PM-011: A Herbal Approach to Breast Cancer: Cytotoxic Studies on *R. Arboreum nilagiricum*

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Breast cancer remains one of the most prevalent and deadly malignancies among women globally, with significant challenges in treatment due to toxicity, drug resistance, and limited specificity. In search of alternative therapies with improved safety and efficacy, this study investigates the anti-breast cancer potential of *Rhododendron arboreum nilagiricum* leaf extract. The plant was authenticated, standardized, and extracted using a hydroalcoholic maceration method. Phytochemical screening revealed the presence of alkaloids, flavonoids, glycosides, phenols, terpenoids, steroids, and other bioactive constituents. In vitro cytotoxicity was assessed using the MTT assay on MCF-7 breast cancer cell lines across a concentration range of 6.25–100 µg/ml. The extract exhibited a dose-dependent reduction in cell viability, with an LD₅₀ value of 193.83 µg/ml, indicating significant antiproliferative activity. These findings support the therapeutic potential of *Rhododendron arboreum nilagiricum* in breast cancer treatment, likely due to its rich phytochemical profile. This study highlights the promise of this traditionally used medicinal plant as a natural cytotoxic agent, warranting further investigation for its mechanisms of action and clinical relevance. Incorporating such plant-based agents could contribute to the development of safer, more effective cancer therapies with fewer adverse effects.

Key words: *Rhododendron arboreum nilagiricum*, Breast cancer, MCF-7 cell line, Cytotoxicity, MTT assay, Phytochemicals, Herbal anticancer agents.

PCO-PM-012: Formulation and evaluation of antifungal soap

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Millions of people worldwide suffer from fungal skin diseases like those caused by *Candida albicans* and dermatophytes, which raises the need for safe, plant-based remedies. The seed oil of *Jatropha curcas*, a plant with antifungal, antibacterial, and anti-inflammatory qualities, is a promising natural ingredient for antifungal personal care products since it is abundant in phytochemicals such flavonoids, tannins, saponins, and phorbol esters. Aim of our formulation is to develop antifungal soap using the seed oil of *Jatropha curcas*, which is primarily intended to treat fungal infections like tinea capitis, a contagious fungal illness of the scalp that primarily affects youngsters and is marked by itching, scaling, and hair loss. To prepare the antifungal soap, glycerine soap base was melted below 60°C using a water bath. Then, *Jatropha curcas* seed oil, aloe vera, and Vitamin E were added and stirred. After slight cooling, citronella perfume was mixed in. The mixture was poured into molds and left to harden at room temperature. The prepared antifungal soap was evaluated for physical characteristics, pH, moisture content, TFM, saponification value, ethanol-soluble matter, foaming index, foam retention, and antifungal activity. These parameters confirmed the soap's effectiveness against fungal infections, as well as its stability and overall cleansing efficiency. Compared to conventional therapies, the herbal soap exhibited favorable physicochemical properties and promising antifungal activity, particularly at higher concentrations. The research presented here emphasizes how skin irritation from synthetic compounds can be reduced by adopting natural and herbal substitutes in personal care products.

Keywords: *Jatropha curcas* seed oil, Antifungal soap, Tinea capitis, Fungal infections



PCO-PM-013: Cannabis-Enriched Polyherbal Formulation for Post-Chemotherapy Care: Clinical Insights and Future Prospects

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Background: Cancer is a multifaceted condition that contributes to 1 in 6 deaths globally. Conventionally, this disease is treated with radiation or/and chemotherapy, which is often associated with debilitating side effects such as pain, immune suppression, gastrointestinal disturbances, and fatigue.

Aims & Objective: The current research attempts to present the therapeutic potential and clinical relevance of a cannabis-based polyherbal formulation in improving the quality of life among post-chemotherapy cancer patients.

Methodology: Extracts of *Cannabis sativa* L. Leaves have shown promising effects in alleviating most of these side effects, making them a safer option. In Ayurveda, 191 formulations are presented in various classical texts to be dispensed in 13 different dosage forms, alongside some proprietary medicines. The developed formulation integrates raw leaf extracts of *Cannabis sativa* L., which is rich in Cannabidiol (CBD) and has a low concentration of Tetrahydrocannabinol (THC), along with herbs like *Tinospora cordifolia*, *Semecarpus anacardium*, *Asparagus racemosus*, *Clerodendrum infortunatum*, and *Simarouba glauca*. The formulation is prepared based on Ayurvedic principles prescribed for Ghrita preparation. Clinical insights from observations on patient volunteers towards use of the formulation post-chemotherapy are provided as case study reports.

Results: The formulation exhibits a significant effect by improving the quality of life through relief from nausea, appetite stimulation, reduced pain, improved sleep and decreased fatigue. Insights from the scientific publications suggest neuromodulation, rebalance of the endocannabinoid system and even apoptosis of cancer cells. The formulation promises to be a safe and effective palliative treatment for post-chemotherapy care.

Conclusion: Its integration with traditional technical knowledge and modern cannabinology science offers a unique multidimensional approach. Further, controlled clinical trials will aid in the establishment of the therapeutic efficacy enhancing patient care.

Keywords: *Cannabis sativa*, CBD, Cancer, Oncology, Ayurveda, Palliative care, Polyherbal.



PCO-PM-014: In Silico Screening of *Bryophyllum pinnatum* Phytochemicals for Targeting Kidney Stone Formation via Crystal Protein Interaction Inhibition

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Background: Kidney stones, particularly the calcium oxalate (caox) varieties, form when urine becomes oversaturated with calcium and oxalate. Once urine becomes oversaturated, it creates a problem by initiating the growth of tiny crystals that clump together, stick to the lining of the kidney, and eventually form stones that can be quite painful. *Bryophyllum pinnatum* is a traditional medicine that has been used in the treatment/prevention of kidney stones. The susceptible factors of this plant includes flavonoids and polyphenols.

Aims & Objectives: To explore, using computer simulations, how key compounds from *Bryophyllum pinnatum*—namely quercetin, kaempferol, and bryophyllin A—might block the proteins that drive calcium oxalate crystal formation and aggregation.

Methods:

1. Selection and Preparation of Phytochemicals

Selection of phytoconstituents identified in *Bryophyllum pinnatum* includes quercetin (pubchem CID: 5280343), kaempferol (pubchem CID: 5280863), and bryophyllin A based on available literature for anti-urolithiatic activity documentation. 3D structures of phytoconstituents will be retrieved through pubchem and prepared for docking through energy minimization and protonation at physiological pH (7.4) using lineage preparation tools.

2. Target Protein Selection and Preparation

The selection of proteins involved in soluble calcium oxalate crystal nucleation and renal inflammation will be potential targets. Proteins include osteopontin (alphafold ID: AF-P10451-F1), annexin A1 (PDB ID: 1HM6), and interleukin-1 β (PDB ID: 5R8J). The protein structures will be cleaned by removing miscellaneous molecules, and then subsequently prepared for docking using the protein preparation wizard.

3. Molecular Docking

The molecular docking will be performed using autodock Vina to predict binding affinity and interaction modes of selected ligands and target proteins. The output of molecular docking will be analyzed to assess the specific amino acid residues involved in binding and select ranked ligand-target complexes based on binding energy.

Molecular Dynamics (MD) Simulations

The ligand-protein complexes (top-ranked molecular docking results) will be subjected to molecular dynamics simulation in GROMACS. The molecular dynamics simulation will be conducted using physiological conditions (300 K, 0.15 M NaCl) to examine the structural stability of the complex over time. Each simulation will be analyzed by root mean standard deviation (RMSD), hydrogen bonding, and stability of the protein-ligand interaction.

ADMET

Drug-like properties—absorption, distribution, metabolism, excretion, and toxicity—were evaluated using swissadme and pkcsim to ensure promising hits also show favorable pharmacokinetics.

Profiling

Results:

We anticipate identifying one or more *Bryophyllum* compounds that:

- Bind strongly and specifically to caox-promoting proteins
- Remain stably attached throughout MD simulations



- Exhibit favorable ADMET characteristics

These findings will highlight the most promising phytochemicals for further laboratory testing against kidney stones.

Conclusion: This study outlines a clear, stepwise in silico approach to predict how *Bryophyllum pinnatum* compounds might prevent calcium oxalate crystal formation. By pinpointing the best candidates, it lays the groundwork for experimental validation and supports the development of plant-based therapies for kidney stone prevention.

Keywords: *Bryophyllum pinnatum*, renal calculi, molecular docking, molecular dynamics simulation, osteopontin, calcium oxalate, ADMET, phytochemicals, antiurolithiatic, pharmacognosy



PCO-PM-015: Anti-Harassment Herbal Spray: A Novel and Natural Approach for Self-Defense

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Background

Women's safety remains a pressing global issue, necessitating innovative solutions for self-defense. Conventional self-defense tools often rely on synthetic chemicals, causing potential health hazards. This study introduces a novel herbal formulation designed as an anti-harassment herbal spray, providing a safe, effective, and eco-friendly alternative for personal protection. To develop and evaluate an herbal spray that temporarily incapacitates attackers using plant-based ingredients, ensuring non-toxic, immediate deterrence without lasting harm.

Aims & Objectives

Aims:

- To develop a natural deterrent against harassment and assault.
- To empower women and vulnerable individuals with enhanced security and confidence.

Objectives:

- To reduce incidents of harassment and assault through safe and effective intervention.
- To increase personal safety and promote widespread use of natural self-defence products.
- To make all women feel safe and efficient in society without afraid of harassments

Methods: A mixture of few herbs used in this formulation combinly shows libido-suppressing, neuroblocking, irritant, and muscle-contractile effects (approximately for 2 to 3 hrs) were dried and ground into a powder. Concentrated bioactive components were obtained by Soxhlet extraction based on ethanol. In order to create a stable spray, the extract was mixed with ethanol and preservatives after undergoing solvent evaporation. For portability, the solution was packaged in atomizer bottles. To standardize production, a formulation table that listed every ingredient and its purpose was made.

Conclusion: The anti-harassment herbal spray is a ground-breaking invention that uses natural methods to promote personal safety. It embodies a vision of women's empowerment that goes beyond its technical capabilities. To increase production and carry out additional preclinical and clinical testing, financial backing and ethical approval are required.

Keywords: Herbal spray, self-defence, women's safety, natural deterrent, personal security



PCO-PM-016: Turmeric For The Prevention Of Viral & Bacterial Pandemics: A Scientific Perspectives

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From time immemorial, turmeric and coconut have been used in Bharat and Southeast Asia. Coconut oil, coconut milk, and turmeric, a golden spice, are widely used in India every day in large quantities for the preparation of curries, pickles, dishes, and sweets. Turmeric and coconut are considered auspicious, used on occasions such as religious and marriage ceremonies. Coronavirus (COVID-19) spreads very quickly and kills people around the world. The mutation rate is very high and happens quickly. The possible way to overcome this disease is to avoid exposure to infected subjects, wash hands frequently with soap, and improve the host's immunity to the virus.

In 1984, Dr. Nagabhushan first published a scientific study to show that turmeric and curcumins prevent genetic damage induced by environmental and dietary mutagens/carcinogens. Consumption and application of turmeric/curcumins may prevent many types of cancer, including skin cancer, leukemia, lymphoma, breast cancer, and stomach cancer (Nagabhushan, 1987). Turmeric in the diet prevents virus-induced spontaneous mammary tumors in mice. Epstein-Barr Virus (EBV) causes lymphoma in humans, and curcumins blocks the EBV activation, proliferation, and transformation of Human B-lymphocytes (1997). In vitro, Curcumins exhibits antiviral activity against papillomavirus, HIV, Ebola, norovirus, chikungunya virus, dengue fever, Zika virus, influenza, and hepatitis B and C virus. Recent molecular docking studies revealed that Curcumins are potential inhibitor of COVID-19 (2020). Virgin coconut oil (VC) has lauric (47%), caproic (7%) and medium chain fatty acids, that exhibit antiviral activities by stimulating the cells to secrete 10 times more triacyl glycerol that will not allow viral protein to assemble properly and make it inactive (e.g. H5N1 virus), Both turmeric/curcumins and VC boost immunity in humans. Various ways of using turmeric and VC will be discussed to prevent viral/bacterial pandemics, such as washing hands, nasal drops, drinking turmeric in milk, body application, and disinfecting with turmeric smoke.



PCO-PM-017: Phytochemical Constituents and Therapeutic Potential of *Sechium edule* (Chayote): An Integrative Review

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Background: The *Sechium edule* (chayote) is a perennial climber of Cucurbitaceae family, which is grown in tropical or subtropical areas such as India, Mexico and Brazil. It is a well-known nutritious and medicinal plant which is used as food with edible fruits, shoots, and roots. It is rich in fiber, amino acids, vitamins and minerals as well as various bioactive compounds such as flavonoids, alkaloids, cucurbitacins, saponins and phenolic acids which make it have long tradition in management of hypertension, diabetes, digestive disorders, nervousness and kidney stone.

Aims & Objectives: To discuss and synthesize the phytochemical constituents and pharmacological potentials of *Sechium edule* based on the possible aspects as a source of bioactive medicinal compounds.

Methods: A literature review was also done integrating the cultivation of the plant, its structure, phytochemical composition and pharmacological aspects.

Results: Phytochemical properties show a lot of flavonoids, alkaloids, saponins, carotenoids, cucurbitacins and minerals. Literature indicates that it possesses numerous pharmacological actions like antioxidant, antihypertensive, antidiabetes, hepatoprotective, antiulcers, antimicrobial, and anti-inflammatory. Conventional applications include remedies against nervousness, headaches of high grade and urinary problems and kidney stones as well as in cosmetics and personal care.

Conclusion: *Sechium edule* is an excellent nutritionally wealthy and pharmacologically diverse plant that has proved to have therapeutic effects. This together with its comprehensive range of biologically active components and proved therapeutic actions makes it into a potential candidate to becoming a contemporary phytomedicine, and future research and clinical trials are to be considered.

Keywords: Chayote, *Sechium edule*, Phytochemistry, Pharmacology, Medicinal plant.



PCO-PM-018: Polyherbal Formulations as Natural Therapeutics in Diabetes Mellitus: a Biological Pathway Based Systematic Review.

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Background: Diabetes Mellitus (DM) is a significant global health problem due to its many consequences. DM leads to many complications which include, retinopathy, bone strength weakness, nephropathy, neuropathy, several cardiovascular diseases, etc. Which later could increase and harm body severely. Conventional treatments for this condition involve prescribing synthetic medications for a brief period that can have negative effects on the body. These drugs have their own negative effects on health. Medicines like, thiazolidinediones, are associated with the risk of fluid retention, bone loss, and congestive heart failure while, SGLT2 inhibitors, such as dapagliflozin, result in bone weakening, urinary tract infection.

Aims & Objectives: This review explores the potential of polyherbal formulations (phfs) made from herbal extracts as an alternative treatment for diabetes. It emphasizes the similarities in mechanism of phfs and synthetic drug, importance of herbal extracts that target biological pathways involved in diabetic human, and highlighting the anti-diabetic effects of phfs, such as reducing oxidative stress, controlling hyperglycaemia, and lowering LDL and proinflammatory cytokines.

Methods: A systematic literature review was conducted across wide scientific data bases between years 2019 to 2024.

Results: phfs like, GTF-231, GP/PROD/2021/001, liberin, Panchavkal, COV, DB14201, glycacare-II, G400, Mehani, etc., have successfully shown anti-diabetic effects with minimal toxicity. Extracts from phfs such as *Tinospora cordifolia*, *Mormodica charantia*, *Gymnema sylvestre*, etc showed significant therapeutic potential through multiple diabetic pathways, such as GLUT4 translocation, AGE/RAGE axis, PI3K/Akt, AMPK etc. For example, *Mormodica charantia* inhibits the activity of alpha-amylase and alpha-glucosidase enzymes thereby reduces the absorption of glucose.

Conclusion: phfs exhibit fewer side effects compared to conventional drug. The mechanism of action of the phytochemicals included in the phfs is similar to that of synthetic medicines. As a result, phfs have the potential to replace synthetic medications while posing less risk to the body. Further research must be done to exploit full potential of phfs in managing DM.

Keywords: Diabetes mellitus, polyherbal formulation, AMPK pathway, Wnt pathway, *Tinosporacordifolia*, phytochemicals.

Category 5

Pharmacology and Biotechnology



PHA-BT-001: Comprehensive In Vitro and In Vivo Assessment of Spermicidal Potential of Ethanolic Bark Extract of *Acacia concinna* in Human Semen and Male Wistar Rats

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Background: Synthetic spermicides may irritate mucosa and elevate infection risk. *Acacia concinna*, a saponin-rich herb used traditionally, remains unexplored for its potential spermicidal activity.

Aims & Objectives: The present study evaluated the spermicidal efficacy of the ethanolic extract of *Acacia concinna* bark using human semen in in vitro assays and vivo experiments using Wister albino rats.

Methods: Ethanolic extract of *Acacia concinna* bark (EEAC) was prepared by hot percolation using a Soxhlet apparatus. In vitro spermicidal activity was assessed by evaluating sperm motility and viability, and EC₁₀₀ was determined. For in vivo analysis, fertile male Wistar rats received EEAC (200 and 400 mg/kg, p.o.) For 28 days. Mating was conducted from day 29 to 35. On day 35, blood was collected for biochemical evaluation, and reproductive organs were weighed. Histopathological examination was subsequently performed.

Results: *In vitro* study demonstrated a dose-dependent reduction in sperm motility, sperm motility reached 0% within 5 minutes at EC₁₀₀ value of 75mg/ml and The extract had minimal impact on sperm viability. Additionally, investigation of sperm morphology using Quick diff staining technique revealed no alterations to the sperm head, mid-piece, or tail morphology in comparison to untreated sperm. To confirm the in vitro findings, in vivo study was conducted, which showed that not a single rat became pregnant when male rats were treated with both the doses of EEAC, indicates a Striking impact on fertility. Histopathological observations further supported these results, revealed closely packed seminiferous tubules, decreased Leydig cells and germ cells, and Lumen lacked spermatozoa in the treated groups, in contrast to the untreated group.

Conclusion: It was concluded that EEAC possessed promising spermicidal effect, which might be because of presence of saponin (lupeol) in the extract which act on catsper. It led to sperm immobilization, reduction in testicular and epididymal weight, and hormonal suppression.

Keywords: Spermicidal, *Acacia concinna*, Testosterone, Antifertility, Reproductive hormones and saponin.

PHA-BT-002: Evaluation of a Mucoadhesive Gel Containing *Cocculus hirsutus* for Colon Cancer Therapy

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Background: Colon cancer is a leading cause of cancer-related deaths worldwide, demanding the development of targeted, effective, and safe treatment strategies. Mucoadhesive gels offer localized drug delivery with improved retention and reduced systemic side effects. *Cocculus hirsutus*, a medicinal plant, contains bioactive mucilage with potential mucoadhesive and therapeutic properties. This study explores its application in formulating a rectal gel for colon cancer treatment.

Aims and Objective: To develop and evaluate a mucoadhesive rectal gel incorporating *Cocculus hirsutus* mucilage, focusing on its physicochemical characteristics, mucoadhesion, safety profile, and anticancer potential for colon cancer therapy.

Methods: *Cocculus hirsutus* leaves were authenticated, and mucilage was extracted using acetone, yielding a higher concentration (1.1%) compared to ethyl alcohol (0.7%). Rectal in situ gels containing 3-Quinucidinone hydrochloride were formulated using Poloxamer-407, Carbopol, and *Cocculus hirsutus* mucilage at varying concentrations. Formulations were evaluated for pH, viscosity, gelation temperature, and mucoadhesive strength. FTIR analysis confirmed no chemical interaction between drugs and polymers. Among the formulations, F10 (with mucilage) showed a gelation time of 1.5 minutes and maintained integrity for up to 1 hour.

Results: Formulations containing *Cocculus hirsutus* mucilage exhibited enhanced gelation and mucoadhesive properties. Rectal irritation studies confirmed the gel's safety. Anticancer activity was evaluated using MTT assays on HT-29 colon cancer cell lines and in vivo in rats with induced colon cancer. Treated groups showed improved hematological parameters, reduced colon and spleen weights, increased antioxidant levels, and better histopathological profiles, indicating effective therapeutic action.

Conclusion: The *Cocculus hirsutus* mucilage-based mucoadhesive gel demonstrated promising results for colon cancer treatment, showing strong mucoadhesion, favorable gelation characteristics, and significant anticancer potential. These findings support its further development as a sustained-release, rectal drug delivery system for colorectal cancer therapy.

Keywords: *Cocculus hirsutus*, Mucoadhesive gel, Colon cancer, In situ gel, 3-Quinucidinone hydrochloride, Mucilage, Mucoadhesion, Sustained release



PHA-BT-003: Antiulcer activity of Ethanolic extract of leaves of *Simarouba glauca* in Wistar albino rats

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Background: Peptic ulcer disease, a condition involving lesions that breach the stomach lining and extend into the submucosa, is largely attributed to a disruption between corrosive elements (like gastric acid and pepsin) and the body's defensive barriers. Traditionally, *Simarouba glauca* leaves have been employed in folk remedies to address ulcer-related symptoms, suggesting therapeutic potential.

Aims & Objectives: This research aimed to explore the gastroprotective properties of an ethanolic extract from *Simarouba glauca* leaves (EESG) using Wistar albino rats as the experimental model.

Methods: The extraction process utilized ethanol in a Soxhlet apparatus to derive active constituents from *Simarouba glauca* leaves. Two experimental protocols-pylorus ligation and swim stress-induced ulcer models were employed to assess the extract's effects at 200 mg/kg and 400 mg/kg dosages.

Results: EESG administration resulted in a statistically significant decrease in gastric secretion volume, total and free acidity, and ulcer severity index ($p < 0.05$). Additionally, a marked elevation in gastric pH indicated reduced acidity and improved mucosal defense.

Conclusion: The study affirms the antiulcer efficacy of *Simarouba glauca* leaf extract, likely owing to bioactive compounds such as quercetin, apigenin, and luteolin. These phytochemicals may underpin its protective and acid-modulating mechanisms, aligning with its traditional medicinal applications in ulcer care.

Keywords: *Simarouba glauca*, Quercetin, Pylorus ligation, Swim stress and Antiulcer activity.



PHA-BT-004: Exploring an anticancer Intra-Vaginal Nano Sponges Containing the Isolates of *Ganoderma Lucidum* in Experimentally Induced Ovarian Cancer Using *in Vivo* Experimental Model

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Background: Ovarian cancer is one of the most lethal gynecological malignancies, usually diagnosed at late stages with unfavorable prognosis and low response to treatment. Natural compounds and targeted drug delivery systems are gaining importance for enhancing therapeutic benefits with reduced side effects.

Aims & Objectives: The present study was undertaken to assess the anticancer potential of an intra-vaginal delivery system of bioactive isolates of *Ganoderma lucidum* encapsulated nano sponges in the in vivo model of experimentally induced ovarian cancer.

Methods: Nano sponges were loaded with bioactive isolates of *Ganoderma lucidum* and delivered intra-vaginally to chemically induced ovarian cancer-bearing female Wistar albino rats. Parameters assessed included antioxidant activity (SOD, catalase, GSH), hematological profile (hemoglobin, RBC, WBC), and histopathological assessment of ovarian tissues.

Results: *Ganoderma lucidum*-loaded nano sponges treatment greatly improved antioxidant levels, reflecting decreased oxidative stress in cancer-bearing rats. Hematological profiles improved with almost normalization of hemoglobin, RBC, and WBC levels, reflecting systemic and immune recovery. Histopathology demonstrated significant tumor regression, reduced cellular proliferation, and regained ovarian tissue architecture from untreated controls.

Conclusion: Intra-vaginal *Ganoderma lucidum* nano sponges exhibited robust therapeutic efficacy by treating ovarian cancer locally, enhancing antioxidant protection, re-establishing hematologic equilibrium, and reversing histological alterations caused by tumors. Such a localized, non-surgical route is a potential novel strategy for cancer treatment.

Keywords: Ovarian cancer, *Ganoderma lucidum*, nano sponges, intra-vaginal delivery, in vivo model.



PHA-BT-005: Colorimetric Detection of Bacterial Contamination in Raw vs. Pasteurized Milk Using Sudan III-Based Indicator Strips

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Background: Milk is an essential dietary component globally but is prone to bacterial contamination, compromising safety despite pasteurization. Standard microbiological assessments are time-consuming and inaccessible in resource-limited settings.

Aims & Objectives: This study aimed to develop a rapid, cost-effective, and colorimetric detection method using Sudan III-treated strips to identify bacterial contamination in raw and pasteurized milk by targeting surface lipoproteins.

Methods: Raw milk samples were aseptically collected, cultured using spread and pour plate techniques, and subjected to microbial isolation and Gram staining. Surface proteins, including lipoproteins, were extracted and applied to filter paper strips pre-treated with Sudan III dye. Comparative colorimetric responses were evaluated for raw vs. Pasteurized milk under both visible and UV light.

Results: Seven distinct bacterial strains were isolated, predominantly Gram-negative rods. Colorimetric analysis using Sudan III showed strong orange-red staining in raw milk samples, indicating high lipoprotein content. Pasteurized milk showed significantly reduced or no staining, suggesting effective microbial reduction but incomplete lipid elimination.

Conclusion: Sudan III-based indicator strips demonstrated potential as a visual biosensor for detecting bacterial contamination through surface lipoprotein interaction. This technique provides a simple and rapid alternative for milk quality assessment, particularly valuable in low-resource environments.

Keywords: Sudan III, milk contamination, lipoproteins, colorimetric assay, pasteurization, biosensor



PHA-BT-006: Exploring the Anti-Parkinson Activity of Kojic Acid on the Zebrafish Model

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Background: Parkinson's disease (PD) is a progressive neurodegenerative disorder characterized by the loss of dopaminergic neurons in the substantia nigra, leading to tremors, bradykinesia, and postural instability. Current treatments focus primarily on symptom management rather than disease modification. Kojic acid (KA), a natural metabolite produced by *Aspergillus oryzae*, has shown neuroprotective effects in Alzheimer's models but remains unexplored in PD. The zebrafish (*Danio rerio*), due to its genetic similarity to humans and well-characterized central nervous system, is a suitable model for PD studies.

Aims & Objectives: To investigate the neuroprotective potential of Kojic acid in a rotenone-induced zebrafish model of Parkinson's disease, with behavioral, biochemical, and histopathological assessments.

Methods: Zebrafish were divided into six groups: Normal, Positive control, Standard (Levodopa), and Kojic acid-treated (5, 10, and 20 mg/L). PD was induced using rotenone (5 µg/L). KA was administered for 28 days. Behavioral parameters were recorded using ANY-maze software. On day 29, fish were euthanized, and brains were harvested for histopathological and biochemical analyses, including ache, SOD, Catalase, and Glutathione assays.

Results: The 10 mg/L KA-treated group demonstrated significantly improved locomotor activity and anxiety-related behavior compared to the positive control. Biochemical assays revealed improved antioxidant enzyme levels and reduced oxidative stress markers. Histopathological findings supported neuronal protection in the KA-treated brains.

Conclusion: Kojic acid, particularly at 10 mg/L, exhibited promising neuroprotective effects in the zebrafish PD model, suggesting its potential as a therapeutic candidate for Parkinson's disease. Further investigations in higher models are warranted to confirm its efficacy and mechanism of action.

Keywords: Parkinson's disease, Kojic acid, Zebrafish, Neuroprotection, Rotenone, Antioxidants



PHA-BT-007: The comparative analysis between rotenone-induced model and the uas gal4 system a30p strain for studying motor and behavioural phenotypes in parkinson's disease in drosophila melanogaster.

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Background: Parkinson's disease stands out as one of the most prevalent and debilitating, characterized by progressive motor dysfunction, cognitive impairment, and a myriad of non-motor. *Drosophila melanogaster* has emerged as a powerful model organism for studying Parkinson's disease, owing to its genetic tractability, short lifespan, and well-characterized nervous system. Rotenone is a pesticide that inhibits mitochondrial complex I, leading to oxidative stress and dopaminergic neuron degeneration, mimicking sporadic PD. This model is widely used to study the environmental factors contributing to PD. In *Drosophila*, exposure to rotenone results in motor and non-motor deficits. Comparatively, expressing human disease and gene-associated proteins in *Drosophila* neurons, researchers can recapitulate key aspects of neurodegenerative pathology using UAS GAL4 system and investigate disease mechanisms in a controlled experimental setting. Notably, transgenic *Drosophila* models harbouring the A30p mutation in the α -synuclein gene have been instrumental in elucidating the cellular and molecular consequences of α -synuclein dysfunction which can be studied and compared with chemical induced model using locomotor assay and courtship assay, which helps in identifying potential therapeutic targets based on pathogenesis for both sporadic and familial PD.

Keywords: *Drosophila melanogaster*, α Synuclein, Geotaxis, A30p mutation, Rotenone, UAS GAL4 system.



PHA-BT-008: Pharmacological and phytochemical investigation of ethanolic extract of *tridax procumbens* linn using in-silico and ex-vivo screening models

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The primary goal in treating chronic illnesses is to manage the condition effectively while minimizing adverse effects. The World Health Organization (WHO) supports the use of herbal remedies for managing long-term diseases. In this context, *Tridax procumbens* Linn., a plant known to contain flavonoids with natural anti-allergic properties, was selected for investigation. This study focuses on evaluating the anti-allergic activity of the plant's ethanolic extract (EETP) using *in-silico* and *ex-vivo* methods. The aerial parts of *Tridax procumbens* were coarsely powdered and extracted with ethanol using a rotary shaker. Phytochemical screening and GC-MS (Gas Chromatography-Mass Spectrometry) analysis were performed to identify the active constituents, revealing 101 compounds. *In-silico* studies using autodock 4.2 identified compounds with strong binding affinities toward allergic reaction-related proteins. *Ex-vivo* studies assays were carried out to assess the extract's ability to inhibit histamine and acetylcholine release, markers of anti-allergic and anti-cholinergic activities. Results showed the ethanolic extract had high flavonoid content, a significant extractive value, and low fluorescence. *In-silico* studies using autodock 4.2 identified compounds with high binding affinities ranging from -4 to -8 kcal/mol toward allergic reaction-related proteins. *Ex-vivo* studies indicated a clear dose-dependent response at 100 mg, 500 mg, and 1000 mg concentrations. These findings suggest that EETP has promising anti-allergic potential. Further in-vitro studies are recommended to confirm its efficacy and explore its use as a natural therapeutic agent for allergic conditions.

Key words: *Tridax procumbens*, Phytoconstituents, GCMS, *Ex-vivo*, *In-silico*, Flavonoids, Anti-cholinergic, Anti-histaminic.



PHA-BT-009: Modeling type 2 diabetes in rats using low protein diet and streptozotocin

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Background: The association between protein malnutrition and type 2 diabetes mellitus (T2DM) is well documented in clinical studies. However, an animal model mimicking the clinical condition of T2DM is not available.

Aims & Objectives:

Aim: To develop a new model of T2DM in rats using low protein diet and streptozotocin.

Objectives:

1. To develop protein-malnutrition rat model.
2. To assess the susceptibility of protein-malnourished rats to streptozotocin mediated diabetes mellitus.

Methods: Male Wistar rats from weaning were fed either a low-protein diet (MB diet, 10% protein) to induce malnutrition or a standard pellet diet (18% protein) as a control. After establishing malnutrition, different doses of streptozotocin (STZ) were administered to induce diabetes in a separate set of animals. Fasting blood glucose was measured 72 hours post-STZ and monitored weekly. At the end of the study, an oral glucose tolerance test was performed. Serum insulin, C-peptide, lipid profile, liver enzymes, BUN, and creatinine were analyzed. Rats were euthanized to collect the pancreas for histopathological evaluation.

Results: Protein-malnourished animals challenged with STZ show the cardinal signs of diabetes. FBG was increased in malnourished groups with an increase in STZ dose compared to the normal control group. Increased OGTT & HOMA-IR values indicate impaired glucose tolerance in these animals. Further, hyperinsulinemia and dyslipidemia confirm insulin resistance. Both liver and kidney functional parameters were high in these animals. Histopathology of the pancreas further confirms these findings.

Conclusion: Results from our study confirm the development of a new model of T2DM.

Keywords: Animal model; HOMA-IR; Type 2 Diabetes mellitus; Protein malnutrition; Low protein diet; Streptozotocin.



PHA-BT-010: Screening of anti-inflammatory activity of leaf extracts of *elaecarpus serratus* L.

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Background:

The tropical flowering tree *Elaeocarpus serratus* is a member of the *Elaeocarpaceae* family. People regularly consume the fruit of the tree, and it is also utilized in traditional medicine. It is also known as Ceylon olive. Traditionally, *E. Serratus* has been used to treat various disease conditions, including piles, jaundice, liver diseases, gastritis, ulcer, fungal infection, joint swelling, toothaches, diarrhoea, and dysentery.

Aims & Objectives: The aim of this study is to investigate the effect of aqueous and ethanolic extract of *Elaeocarpus serratus* L. For their anti-inflammatory activity using animal models.

Methods: Phytochemical analysis was carried out according to standard procedure as mentioned to detect the major chemical constituents. In the present study assessed the following Pharmacological activity using animal experimental models.

Anti-inflammatory activity: The effect of different extract of *Elaeocarpus serratus* was investigated by employing two models i.e. Carrageenan induced hind paw edema and Formalin induced paw edema model. Indomethacin and Diclofenac sodium were taken as reference standard drug respectively.

Results: The phytochemical investigations revealed the presence of Flavonoids, Carbohydrates, Proteins, Tannins, Saponins, Triterpenoids, Steroids, Glycosides and Alkaloids. The result of experimental data revealed that, the ethanol and aqueous extracts of leaf of *E. Serratus* at dose 400mg/kg shows significant and moderately significant in Anti-inflammatory activity.

Conclusion: The outcome of this study provides evidence that the ethanol and aqueous extracts of *E. Serratus* possess significant and moderately significant Anti-inflammatory activity. The activities may be due to the presence of phytochemicals like Flavonoids, Tannins, Glycosides and Alkaloids in test extracts.

Keywords: *E. Serratus*, Indomethacin, Diclofenac sodium, Anti-inflammatory, Flavonoids.



PHA-BT-011: Advanced Scaffolds for Diabetic Wounds: A Formononetin NLC Approach

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Diabetic individuals exhibit a reduced capacity to metabolize glucose, leading to hyperglycaemia, which further complicates the wound healing process. Diabetic foot ulcers affect approximately 34% of the global population. The absence of effective prevention and management strategies has resulted in a growing global incidence of delayed wound healing among diabetic patients. Formononetin (FNMT), a plant-sourced polyphenol, offers therapeutic properties such as antioxidant and anti-inflammatory effects. This study aims to develop Formononetin-incorporated Chitosan-PVA composite scaffolds for treating diabetic wounds. These scaffolds are assessed for physicochemical features, while in-vitro cytotoxicity tests are employed to evaluate cell viability. Furthermore, wound healing efficacy is tested in full-thickness excision wounds using an in-vivo model of streptozotocin-induced diabetic rats. The scaffold formulation is achieved via the freeze-drying method. Parameters such as porosity, water retention, and scaffold degradation are examined. In-vitro drug release analysis showed that 76.7% of formononetin was released within 48 hours, and cytotoxicity assays confirmed safety up to 1000µg/ml of FNMT. In-vivo experiments involved inducing diabetes in rats through an injection of 60 mg/dl of Streptozotocin (STZ) to study wound closure, hexosamine levels, and hydroxyproline content. Hence, FNMT-loaded Chitosan-PVA scaffolds hold promise for diabetic wound management.

Keywords: Diabetic foot ulcers; Formononetin; Chitosan-PVA Scaffolds; Streptozotocin.



PHA-BT-012: Exploring Phytoconstituents for Parkinson's Disease: Insights from Network Pharmacology and Molecular Modelling and *In Vivo* Investigations

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Background: Network pharmacology approach is used to identify novel therapeutic agents that target multiple disease targets through analysis of complex disease networks by integrating systems biology and computational approaches.

Objective: The current study aims to identify the principal targets implicated in the pathogenesis of Parkinson's disease and major phytoconstituents that could potentially modulate the major targets to achieve therapeutic benefits in PD through a network pharmacology-based approach.

Methods: disgenet database was used to select the major targets involved in the pathogenesis of PD. The most important targets among the selected proteins were identified through analysis of topological parameters like degree, betweenness centrality and closeness centrality using Cytoscape software. The phytoconstituents present in the selected botanicals were identified from databases and were subjected to prediction of pharmacokinetic parameters. The binding affinity, free energy and binding stability of the selected phytochemicals with the target proteins were evaluated using molecular docking, MM-GBSA and molecular dynamics respectively using Schrodinger software. The effect of berberine on catalepsy, motor coordination, locomotion and memory were evaluated using rotenone induced PD in rats.

Results: Based on topological parameters and pharmacokinetic profile, 4 proteins (A2A, CNR1, REN and STAT3) and 6 phytoconstituents (berberine, bisacumol, capsaicin, ferulic acid, cinnamic acid and geranyl acetate) were selected respectively for further studies. Among the chosen ligands, berberine exhibited maximum binding affinity with A2A (-9.90 kcal/mol), REN (-7.89 kcal/mol), STAT3 (-3.93 kcal/mol) and second highest with CNR1 (-9.07 kcal/mol). Berberine also showed better free energy scores in MM-GBSA with three targets, A2A (-86.44 kcal/mol), REN (-108.93 kcal/mol), CNR1 (75.18 kcal/mol). The RMSD of berberine with all the four targets in molecular dynamics indicated good ligand-target stability. A significant improvement in catalepsy test, motor coordination, locomotion and memory in animals treated 25 and 50 mg/kg of berberine compared with the control group.

Conclusion: The current network pharmacology-based study reveals that berberine could act as beneficial agent in PD through alteration of multiple receptors.

Keywords: Network pharmacology, Parkinson's disease, berberine, docking, molecular dynamics.



PHA-BT-013: Development of an intravaginal spray containing plant-based medicine for the treatment of ovarian cancer: in vitro and in vivo approaches

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Background: Ovarian cancer is a major cause of cancer-related mortality among women globally, largely due to its asymptomatic nature and diagnosis at advanced stages. Existing therapeutic options, including surgery and chemotherapy, are limited by severe side effects and a high risk of drug resistance.

Aims & Objectives: The present study aims to develop and evaluate an intravaginal spray formulation containing bioactive compounds derived from black wheat (*Triticum aestivum*) for the potential treatment of ovarian cancer.

Methods: The research employed both in vitro and in vivo approaches. Bioactive compounds were extracted from black wheat and formulated into an intravaginal spray. The formulation was characterized and assessed for compatibility. Its safety profile was determined through mucosal irritation studies in accordance with ISO guidelines. In vitro anti-cancer activity was evaluated using selected ovarian cancer cell lines. In vivo efficacy and safety were assessed in rats with DMBA-induced ovarian cancer. Ovarian cancer was induced using DMBA at a dose of 1.5 mg/0.02 ml on the first day, followed by daily administration for 45 consecutive days. Treatment with the test formulation commenced on day 46 and continued for 21 days.

Results: Histopathological and hematological analyses demonstrated that the intravaginal spray significantly reduced tumor size and body weight, improved antioxidant levels, and exhibited minimal systemic toxicity.

Conclusion: The findings suggest that the developed intravaginal spray formulation containing black wheat bioactive compounds holds promise as a safe and effective alternative strategy for the treatment of ovarian cancer.

Keywords: Ovarian cancer, Intravaginal spray, Black wheat, Bioactive compounds, DMBA model, Anti-cancer efficacy.



PHA-BT-014: Transcriptomic Insights into UV-Induced DNA Damage Response in TP53-Mutant Melanoma Cells.

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Background: Melanoma, an aggressive skin cancer, is primarily driven by UV-induced DNA damage. While TP53 mutations occur in only ~20% of melanomas, they are implicated in altered DNA damage responses and resistance to apoptosis.

Aims & Objectives: To investigate how TP53 mutation influences UVB-induced transcriptional and cellular responses in melanoma, particularly regarding apoptosis suppression and survival signaling.

Methods: Transcriptomic profiling (RNA-Seq) was performed on TP53-mutant (A375) and wild-type (SK-MEL-28) melanoma cells post-UVB exposure. Differential gene expression was validated via qrt-PCR and Western blotting. Apoptosis and PI3K/AKT pathway activity were functionally assessed using flow cytometry and pharmacologic inhibition (caspivastib).

Results: UVB exposure led to downregulation of pro-apoptotic genes (BAX, PUMA: $\log_2FC \approx -2.0$, $p < 0.01$) and upregulation of DNA repair genes (XRCC1, PARP1: $\log_2FC > +3.0$). TP53-mutant cells showed significantly elevated PI3K/AKT signaling (p-AKT/AKT $\uparrow$ 8-fold, $p = 0.005$). Apoptosis was markedly reduced in TP53-mutant cells (~60% lower than wild-type), confirming apoptotic evasion. Caspivastib treatment restored apoptosis levels post-UVB exposure.

Conclusion: TP53 mutation in melanoma promotes survival by impairing apoptosis and enhancing DNA repair via PI3K/AKT activation. Targeting this pathway may restore UV sensitivity, suggesting a promising therapeutic approach for TP53-mutant melanoma.

Keywords: Melanoma, TP53 mutation, UV damage, transcriptomics, apoptosis, DNA repair, PI3K/AKT, A375, SK-MEL-28



PHA-BT-015: Genoprotective potential of resveratrol against paraquat induced genotoxicity using Swiss albino mice

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Background: The study investigates how resveratrol (Res), a naturally occurring phytoalexin, protects human lung cells from oxidative damage and fibrosis brought on by paraquat (PQ). PQ, a common herbicide, builds up in the lungs and causes in fibrosis and oxidative damage. Res suppressed the synthesis of profibrogenic and inflammatory factors in normal human lung fibroblasts and markedly decreased PQ toxicity in normal human bronchial epithelial cells. Res also triggered cytoprotective genes via activating the Nrf2 signalling pathway. By activating Nrf2 signalling, Res reduces PQ-induced fibrotic responses, inflammation, and reactive oxygen species formation, the study concluded, exposing a new molecular intervention strategy against pulmonary oxidative damage and fibrosis.

Aim: The aim of the present study is to evaluate the genoprotective potential of Resveratrol against Paraquat Induced Genotoxicity in Swiss Albino Mice.

Objective:

- ❖ To evaluate the genoprotective effect of RSV against PQ induced genotoxicity by Micronucleus assay and Chromosomal aberrations as per OECD guidelines.
- ❖ To evaluate the antioxidant potential of RSV against PQ by determining the tissue LPO levels.

Methods: The experimental protocols are done in accordance with OECD guidelines No.470.

- Animal- Swiss Albino Mice (either sex).
- Age - 6-7 weeks old.
- Weight- 25-30g.
- Genotoxic Dose of PQ-20 mg/Kg body weight.
- Resveratrol- 5mg/Kg body weight.

Results & discussion: PQ induced genotoxicity is intentional or accidental. Studies suggest that antioxidants minimize or counter the effects of genotoxins. This is achieved by reducing. Resveratrol a potent antioxidant, has been studied extensively for its beneficial effects against oxidative stress.

In our study, RSV reversed the effects of PQ induced genotoxicity in bone marrow tissues. The results clearly state that 73.28% reduction in the micronucleus formation and 35.61% reduction in chromosomal aberration. This is supported the LPO inhibition in liver by 20% and lungs by 21.1%. The results suggest that in-built antioxidant mechanisms are also enhanced.

Conclusion: Resveratrol has genoprotective potential against Paraquat induced genotoxicity due to its effective antioxidant activity. It may act as a genoprotective agent against exposure to pesticides when consumed regularly in their natural sources.



PHA-BT-016: A Comprehensive In-Silico Approach for the Functional Prediction and Structural Characterization of snps in the Alzheimer's Disease-Associated PSEN1 Gene
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Background: Alzheimer's disease (AD) is a progressive neurodegenerative disorder marked by cognitive decline and amyloid plaque accumulation. The γ -secretase complex, particularly the Presenilin-1 (PSEN1) protein, plays a critical role in processing amyloid precursor protein (APP). Mutations in the PSEN1 gene are strongly associated with early-onset familial Alzheimer's disease (EOFAD). This study employed integrated computational approaches to investigate the structural, functional, and regulatory impacts of PSEN1 single nucleotide polymorphisms (snps) linked to AD.

Aims & Objectives: To evaluate how pathogenic PSEN1 mutations influence protein stability, structural integrity, post-translational modifications (ptms), gene regulation, and protein-protein interactions to better understand their contribution to AD pathology.

Methods: Functional predictions using SIFT, polyphen-2, and PROVEAN identified snps such as P267S, G206A, and V261A as deleterious. Conservation analysis via consurf confirmed these mutations occur in highly conserved regions, including transmembrane and catalytic domains. Protein stability assessments (I-Mutant 2.0, mupro) revealed a reduction in protein stability ($\Delta\Delta G < 0$). PTM analysis using netphos 3.1a highlighted phosphorylation hotspots in the N- and C-terminal regions affected by snps. Gene interaction mapping with genemania showed PSEN1's interactions with key AD-related genes (e.g., PSEN2, BACE1, MAPT). Regulatory analysis using g:snpsense indicated potential alterations in transcription factor or mirna binding sites.

Results: Deleterious snps were predicted to disrupt conserved domains, reduce protein stability, interfere with phosphorylation regulation, and modulate PSEN1 gene expression. These effects collectively suggest impairment in γ -secretase assembly and APP cleavage.

Conclusion: PSEN1 mutations affect structural stability, regulatory mechanisms, and gene expression, thereby impairing γ -secretase function and contributing to AD pathology. These findings highlight the potential of targeting phosphorylation patterns, stability, and gene regulation in future AD therapies.

Keywords: PSEN1, Alzheimer's disease, γ -secretase complex, Mutations, snps.



PHA-BT-017: Development of a Nasal Spray with Anti-Pro-Inflammatory and Chemotactic Effect for the Management of Pulmonary Fibrosis Using Suitable Experimental Models

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Background: The present study aimed to assess the safety and efficacy of a nasal spray containing synthetic medicine for treating Pulmonary fibrosis. Current treatment strategies, such as anti-fibrotic therapy, often face limitations like severe side effects and the development of drug resistance. Nasal drug delivery systems offer a promising route for localized treatment, providing direct access to the lungs while reducing systemic toxicity. Acute inhalational toxicity studies were conducted by OECD guidelines 403 using rats. Bleomycin was used to induce Pulmonary fibrosis in C57/BL6 Mice. Following induction, treatment with the nasal spray was initiated. At the end of the treatment period, the lungs were isolated and subjected to histopathological and serum biomarkers analysis to assess the formulation's therapeutic efficacy and safety.

Aims & Objectives: The aim of the current study is to prepare the nasal spray for the management of pulmonary fibrosis using suitable experimental models

Objectives

1. To develop a nasal spray formulation by employing appropriate pharmaceutical methods
2. To characterize the developed formulation with suitable parameters to validate and optimize the final formulation
3. To assess the safety of the formulation using standard OECD guidelines
4. To ascertain the potency/beneficial effect of the formulation by *in-vitro* method
5. To evaluate the therapeutic benefits of the formulation by *in-vivo* method in rodents

Methods: This study developed and evaluated a nasal spray for treating Pulmonary Fibrosis. Nasal Spray containing Pirfenidone and Saracatinib was prepared using Tween 80, PEG 400 and distilled water in varying concentrations.

The formulations were assessed for physical properties, pH, viscosity, spray volume, spray pattern and Stability Studies. FTIR studies confirmed no chemical interaction between the drugs and excipients.

Safety for local toxicity and systemic toxicity of respiratory system was ensured through OECD Guideline 403 - Acute Inhalational toxicity studies in animals. The *in-vitro* studies were performed on NIH 3T3 cell lines, and in vivo studies on C57/BL6 Mice induced with Pulmonary Fibrosis.

Results: Serum Biomarkers (TGF-Beta, IL-13) analysis, lung weights, antioxidant levels, and histopathological examinations were assessed. Results suggest that the nasal spray shows potential therapeutic efficacy for Pulmonary fibrosis and demonstrated minimal systemic toxicity.

Conclusion: The developed nasal spray with Pirfenidone and Saracatinib showed promising results for treating pulmonary fibrosis. It was stable, safe, and effective in both *in-vitro* and *in-vivo* models, with minimal toxicity. These findings support its potential as a non-invasive treatment option.

Keywords: Pulmonary Fibrosis, Nasal Spray, NIH 3T3 cell line, TGF-Beta, IL-13



PHA-BT-018: Evaluation of anti-cancer activity of beta-sitosterol from axinella in treating prostate cancer.

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Background: Prostate cancer (pca) is one of the most prevalent malignancies in men, with significant mortality rates globally. Dysregulation of the MDM2-p53 pathway is a crucial molecular event contributing to pca progression. Beta-sitosterol, a phytosterol found in marine sponges such as *Axinella tenudigitata*, has demonstrated various pharmacological activities including anticancer potential. Its role as an inhibitor of the MDM2-p53 interaction suggests therapeutic potential in prostate cancer management.

Objective: To evaluate the anticancer potential of Beta-sitosterol derived from *Axinella* in a rat model of prostate cancer and understand its interaction with the MDM2-p53 pathway using in-silico and in-vivo approaches.

Methods: The study began with computational docking and molecular dynamics simulations to predict how well Beta-sitosterol binds to the MDM2-p53 protein complex (PDB ID: 7BIV). Prostate cancer was then induced in male Wistar rats using testosterone and N-methyl-N-nitrosourea (MNU). Rats were divided into four groups: normal control, disease control, and two treatment groups receiving Beta-sitosterol at 10 mg/kg and 20 mg/kg doses orally for 14 days. Throughout the study, key parameters like body weight, prostate tumor weight, survival time, and tissue histology were closely monitored.

Results: Beta-sitosterol showed a strong binding affinity to the MDM2-p53 complex in silico, suggesting it could effectively block this cancer-promoting interaction. In the animal model, Beta-sitosterol significantly reduced tumor weight, improved survival time, and preserved normal tissue architecture, particularly at the higher dose. The histopathology results confirmed reduced cancerous changes in the prostate tissues of treated rats.

Conclusion: This study highlights the potential of Beta-sitosterol, a natural compound from marine sponge *Axinella*, as a promising candidate for prostate cancer treatment. Its ability to target the MDM2-p53 axis and show tangible benefits in preclinical models encourages further research toward clinical application.

Keywords: Prostate cancer; Beta-sitosterol, *Axinella*, MDM2-p53, in vivo study, natural product, anticancer agent.



PHA-BT-019: Phytochemical and pharmacological evaluation of cucurbita moschata seeds for ischemic stroke.

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Background: Stroke is a serious life-threatening condition caused by an interruption in the brain's blood supply. Linoleic acid, oleic acid, and minerals like magnesium and phosphorus are known for their beneficial effects in preventing and treating stroke.

Aims & Objectives: This study aimed to identify phytoconstituents and evaluate *Cucurbita moschata* seed extract (ECMS) in vitro for stroke. It included phytochemical analysis of ECMS, in vitro testing on an ischemic stroke model using neuroblastoma cells, and in silico evaluation of specific molecular targets.

Methods: *Cucurbita moschata* plants were collected from Pattambi village, Palakkad district, and authenticated. The seeds were shade-dried, coarsely powdered, and extracted via cold maceration using ethanol. ECMS was analyzed for phytoconstituents, fatty acids, and magnesium content using GC-MS and ICP-MS, respectively. In vitro evaluation was done using SH-SY5Y cell lines in a cobalt chloride-induced hypoxia model to mimic ischemic stroke. The MTT assay was conducted to assess cell viability and neuroprotective activity. In silico studies used Schrodinger Maestro 12.8 to evaluate linoleic and oleic acid binding with Prolyl hydroxylase 2 (PDB ID: 5OX6) and Phosphodiesterase 4D (PDB ID: 3G4G).

Results: The ECMS extract yielded 3.604% w/w. Phytochemical analysis showed the presence of carbohydrates, alkaloids, tannins, fatty acids, and flavonoids. Fatty acid profiling revealed a high content of linoleic acid (50.24%) and oleic acid (21.41%) with significant magnesium levels. In vitro studies confirmed ECMS's neuroprotective potential against ischemic stroke. In silico results showed strong affinity of linoleic and oleic acids toward Prolyl hydroxylase-2 and Phosphodiesterase-4D.

Conclusion: ECMS shows protective potential against stroke, likely due to its content of linoleic acid, oleic acid, and magnesium.

Keywords: Ischemic stroke, *Cucurbita moschata*, Prolyl hydroxylase-2, Phosphodiesterase-4D.



PHA-BT-020: Machine Learning-Driven Identification of mirna Biomarkers in Triple-Negative Breast Cancer

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Background: Triple-negative breast cancer (TNBC) accounts for approximately 15% of all breast cancers and is characterized by the absence of targeted therapies. Micornas (mirnas), known for their roles in gene regulation, have emerged as key biomarkers in cancer due to their aberrant expression patterns and non-invasive detectability in human serum. Reliable, non-invasive biomarkers for early TNBC detection remain an unmet clinical need.

Aims & Objectives: To identify circulating serum mirna biomarkers for early detection of TNBC using integrative genomic approaches and machine learning models.

Methods: mirna sequencing data from The Cancer Genome Atlas (TCGA) comprising 150 TNBC samples and 100 control samples were analyzed. Feature selection was conducted using LASSO regression and random forest algorithms. Independent validation was performed using quantitative real-time PCR (qRT-PCR) in an external cohort (n = 50).

Results: Two mirnas—mir-21 (AUC = 0.89) and mir-155 (AUC = 0.85)—demonstrated strong predictive performance with 92% sensitivity in TNBC detection. Both biomarkers were significantly associated with metastasis-free survival (Hazard Ratio = 2.1, p = 0.008).

Conclusion: mir-21 and mir-155 exhibit strong potential as non-invasive, serum-based biomarkers for TNBC screening and prognosis. Their integration into diagnostic workflows could enhance early detection and patient outcomes.

Keywords: Triple-negative breast cancer, mirna biomarkers, LASSO regression, TCGA, AUC



PHA-BT-021: Computational Modeling of Beta-Lactamase Variants in Multidrug-Resistant *Escherichia coli*

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Background: β -Lactamases are major contributors to resistance against β -lactam antibiotics in gram-negative bacteria. The emergence of extended-spectrum β -lactamases (esbls), especially TEM-1 and CTX-M-15 variants, represents a critical challenge in the treatment of multidrug-resistant *Escherichia coli*. These enzymes hydrolyze third-generation cephalosporins and are responsible for widespread resistance. Structural elucidation of these variants is essential for rational inhibitor design.

Aims & Objectives: To predict the 3D structures of TEM-1 and CTX-M-15 beta-lactamases and assess their substrate-binding dynamics for the development of more effective inhibitors.

Methods: 3D structures were predicted using SWISS-MODEL and MODELLER. Molecular docking was conducted using autodock Vina to evaluate binding affinities of ceftazidime and avibactam. Molecular dynamics simulations were performed with GROMACS over 100 ns to investigate structural flexibility and stability.

Results: CTX-M-15 demonstrated broader substrate specificity, associated with increased flexibility in the Ω -loop region (RMSF = 1.8 Å), compared to TEM-1 (RMSF = 1.2 Å). Docking scores indicated higher affinity of avibactam for TEM-1 (-9.2 kcal/mol) than CTX-M-15 (-8.1 kcal/mol), highlighting structural and functional divergence between the two enzymes.

Conclusion: Structural variations between TEM-1 and CTX-M-15 emphasize the necessity for designing dual-target inhibitors. Computational insights provide a foundational basis for future experimental validation in combating ESBL-mediated resistance.

Keywords: Beta-lactamase, Antibiotic resistance, SWISS-MODEL, GROMACS, TEM-1, CTX-M-15.



PHA-BT-022: Gastroprotective Potential of Dark Chocolate in an Experimental Mouse Model of Ulcerative Colitis

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Background: Ulcerative colitis (UC) is a chronic inflammatory bowel disease involving mucosal inflammation, oxidative stress, and gut microbiota imbalance. Recent evidence highlights the role of peripheral dopamine in modulating immune responses and restoring gut homeostasis. Dark chocolate, rich in polyphenols and flavonoids, may offer anti-inflammatory and neuromodulatory benefits via the gut-brain axis.

Aims & Objectives: To evaluate the therapeutic potential of dark chocolate at varying concentrations (85%, 42%, and 21%) in a DSS-induced mouse model of UC, focusing on peripheral dopamine release, inflammation control, antioxidant status, and gut microbiota modulation.

Methods: Male BALB/c mice were administered broad-spectrum antibiotics for 10 days to induce gut dysbiosis. Ulcerative colitis was then induced using 2% dextran sodium sulfate (DSS) for 4 days. Post-induction, mice were treated with dark chocolate of 85%, 42%, and 21% cocoa content for 14 days. Clinical parameters (body weight, colon length, disease activity index), biochemical markers (TNF- α , SOD, catalase, glutathione, dopamine), histopathological assessments, and hematological profiles were evaluated.

Results: Dark chocolate, particularly at 85%, significantly improved clinical outcomes, reduced TNF- α levels, and enhanced antioxidant enzymes (SOD, catalase, glutathione). Elevated peripheral dopamine levels were observed, which correlated with a reduction in inflammation and restoration of gut microbial balance. Histological analysis showed reduced mucosal damage and inflammatory infiltration, while hematological parameters reflected systemic recovery.

Conclusion: Dark chocolate, especially with higher cocoa content (85%), demonstrates strong therapeutic potential in DSS-induced ulcerative colitis by attenuating inflammation, enhancing antioxidant defenses, and modulating the gut-brain axis via peripheral dopamine. It may serve as a promising functional dietary adjunct in UC management.

Keywords: Dark chocolate, Ulcerative colitis, Peripheral dopamine, DSS, Antioxidants, Gut-brain axis.



PHA-BT-023: Unraveling the Effects of Fisetin and Dapagliflozin on DHEA-Induced Polycystic Ovarian Syndrome

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Background: Polycystic Ovarian Syndrome (PCOS) is a common endocrinopathy in reproductive-age women presented with hyperandrogenism, insulin resistance and polycystic ovaries. Present therapy is essentially symptomatic with many limitations and side effects. In the current study, it was hypothesized that Fisetin, a natural flavonoid, which is reported to have antioxidant, anti-inflammatory effects and insulin-sensitizing effects needs to be checked in the context of PCOS therapy and its combination FIST + DAPA in terms of PCOS was investigated.

Objectives: The aim of the study was to evaluate the synergistic curative effects of Fisetin with Dapagliflozin on metabolic, hormonal, and histological parameters in DHEA induced PCOS rat model.

Methods:

- PCOS was established in female Wistar rats by injecting DHEA (60 mg/kg) subcutaneously for 21 days.
- Rats were divided into the following five groups: control, PCOS (DHEA), DHEA+Dapagliflozin, DHEA+Fisetin, and a combination treatment with DHEA+Fisetin+Dapagliflozin.
- The work employed different analytical tools like in silico docking, in vivo biochemical analysis.
- Measured parameters: fasting blood glucose, lipid profile, hormonal profile, antioxidant enzyme activities (CAT, SOD, gpx, TBARS), and inflammatory markers (TNF- α , IL-6).
- Ovarian sections were also subjected to histopathological evaluation.

Results: The results showed that Fisetin and Dapagliflozin and their co-administration significantly restored the disturbed parameters of PCOS rats. PARTICULARLY THEY WERE EFFECTIVE FOR:

- Body weight
- Regularity of estrous cycle
- Hormonal balance
- Lipid metabolism
- Insulin sensitivity
- The combined therapy was superior, remarkably decreasing the oxidative stress and inflammatory indices.
- It also ameliorated the histological structure of the ovary to normal level as denoted by the appearance of corpora lutea and the decrease in the number of cystic follicles.

Conclusion: The results showed that Fisetin+Dapagliflozin was an efficient strategy for improving the metabolic and reproductive disturbances in the DHEA-induced PCOS rat model. This effect is due to suppression of the PI3K/AKT signal pathway and of oxidative stress and inflammation. The results indicate a potential adjunct therapeutic for the control of PCOS.



Keywords: Polycystic Ovary Syndrome (PCOS), Fisetin, Dapagliflozin, DHEA-induced PCOS, Insulin Resistance, Oxidative Stress, Inflammation, PI3K/AKT Pathway, Antioxidant Markers, Hormonal Imbalance, Histopathology, SGLT2 Inhibitor.

PHA-BT-024: Formulation and Evaluation of Chitosan-Based Nanoparticles for Effective sirna Delivery Targeting Aldose Reductase in Neuro2A Cells

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Background: Aldose reductase (AR), the rate-limiting enzyme of the polyol pathway, is overactivated under hyperglycemic conditions, resulting in sorbitol accumulation, oxidative stress, and neuronal injury. Targeting AR expression using small interfering RNA (sirna) is a promising therapeutic strategy for reducing glucose-induced cellular damage. However, the clinical translation of sirna is hindered by its instability, poor cellular uptake, and rapid systemic clearance.

Objective: This study aimed to formulate chitosan-based nanoparticles for efficient delivery of AR-targeting sirna to Neuro2A cells and to evaluate their physicochemical characteristics, cytocompatibility, cellular uptake, and gene silencing efficacy.

Methods: Chitosan–sirna nanoparticles were prepared through electrostatic interaction between chitosan and sirna, without chemical crosslinkers. Particle size, polydispersity index (PDI), zeta potential, and encapsulation efficiency were measured. Cytotoxicity was assessed using cell viability assays, while intracellular sirna delivery was visualized via fluorescence microscopy. RT-PCR was used to quantify AR gene knockdown.

Results: The formulated nanoparticles exhibited a mean particle size of 168 ± 11 nm, PDI of 0.19 ± 0.04 , zeta potential of $+27 \pm 3$ mv, and $>90\%$ sirna encapsulation efficiency. Cytotoxicity analysis demonstrated $>85\%$ Neuro2A cell viability across all tested concentrations, contrasting with significant toxicity observed with lipofectamine. Fluorescence microscopy confirmed intracellular uptake of FITC-labeled sirna. RT-PCR revealed dose-dependent AR silencing, achieving 70–76% knockdown at 50–100 nm sirna concentrations.

Conclusion: Chitosan–sirna nanoparticles provide a safe and effective platform for RNA interference-based therapeutics targeting AR. This delivery system shows potential for treating diabetic neuropathy and other neurodegenerative conditions linked to hyperglycemia-induced neuronal damage.

Keywords:

Chitosan nanoparticles, sirna delivery, Aldose reductase, Neuro2A cells, Gene silencing, Diabetic neuropathy, Polyol pathway, Nanomedicine.



PHA-BT-025: Formulation and evaluation of ethanolic extract of *Dodonaea viscosa* loaded solid lipid nanoparticles against rotenone induced parkinsonism

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Background: Parkinson's disease (PD) is the second most prevalent neurodegenerative disorder after Alzheimer's disease, affecting primarily the elderly population. It is characterized by motor symptoms such as tremors, rigidity, bradykinesia, and postural instability. These symptoms arise due to the progressive degeneration of dopaminergic neurons transmitting signals from the striatum (ST) to the substantia nigra (SN). Identifying effective neuroprotective agents is crucial to managing PD progression. *Dodonaea viscosa*, a plant known for its antioxidant, anti-inflammatory, and cytotoxic activities, has demonstrated potential neuroprotective properties, particularly in rotenone-induced models of α -synuclein aggregation.

Aims & Objectives:

This study aims to investigate the neuroprotective efficacy of *Dodonaea viscosa*-loaded solid lipid nanoparticles in a rotenone-induced rat model of Parkinson's disease by evaluating behavioral, biochemical, and antioxidant parameters.

Methods:

Adult Wistar rats (200–250 g) were subjected to daily intraperitoneal injections of rotenone (3 mg/kg) for 21 days to induce Parkinsonism. From day 7 to day 21, the treatment group received *Dodonaea viscosa* encapsulated in solid lipid nanoparticles. Behavioral tests, including the Open Field Test, Beam Walk, Elevated Plus Maze, and Catalepsy Test, were conducted. Antioxidant enzyme levels (SOD, Catalase, MDA, Glutathione) and acetylcholine esterase activity were measured.

Results: Rotenone administration led to significant oxidative stress and motor dysfunction. Treatment with *Dodonaea viscosa*-loaded solid lipid nanoparticles significantly improved antioxidant enzyme activity, cognitive function, locomotor activity, and memory compared to the untreated group. Behavioral and biochemical evaluations supported the neuroprotective efficacy of *Dodonaea viscosa*.

Conclusion: *Dodonaea viscosa* delivered through solid lipid nanoparticles exhibits promising neuroprotective effects in a rotenone-induced rat model of Parkinson's disease. These findings support its potential role as a therapeutic agent for managing and modifying the progression of Parkinson's disease.

Keywords: Alpha-synuclein, *Dodonaea viscosa*, Lewy bodies, Neurodegeneration, Oxidative stress, Parkinson's disease



PHA-BT-026: Assessment of andrographolide's efficacy in dehydroepiandrosterone-induced PCOS in rats.

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Background: Polycystic Ovary Syndrome (PCOS) is a prevalent endocrine disorder in women of reproductive age, characterized by hormonal imbalance, insulin resistance, oxidative stress, and chronic inflammation. Current pharmacological interventions often have limitations or side effects, prompting interest in plant-based therapeutics.

Objective: This study aimed to evaluate the therapeutic efficacy of andrographolide—a bioactive compound derived from *Andrographis paniculata*—in a rat model of DHEA-induced PCOS, using a combination of in silico and in vivo approaches.

Methods: PCOS was induced in Wistar rats via subcutaneous DHEA administration. Rats were divided into control and treatment groups, receiving andrographolide at 10 mg/kg and 20 mg/kg orally for 21 days. Endpoints included assessment of estrous cyclicity, hormonal levels, lipid profiles, glucose and insulin, oxidative stress markers (SOD, CAT, gpx, TBARS), inflammatory cytokines (TNF- α , IL-6), and ovarian histopathology.

Results: Treatment with andrographolide, particularly at 20 mg/kg, significantly restored regular estrous cycles and normalized body and ovarian weights. Hormonal imbalances and dyslipidemia were corrected, insulin sensitivity improved, and antioxidant enzyme levels were upregulated. Inflammatory markers were notably reduced. Histological analysis revealed reversal of cystic changes and restored follicular development.

Conclusion: Andrographolide demonstrated multi-targeted efficacy in mitigating PCOS features through modulation of oxidative stress, inflammation, and hormonal pathways. Its action on PI3K/Akt signaling suggests a mechanistic foundation for its therapeutic effects. These findings support further exploration of andrographolide as a potential Phyto therapeutic agent for PCOS management.

Keywords: *Andrographolide, PI3K/Akt Pathway, Oxidative Stress, Inflammatory Cytokine.*

PHA-BT-027: Formulation of Stabilized Probiotics for Anti-Aging: A New Approach to Skin Care.

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Background: With growing interest in safe and natural alternatives to synthetic skincare products, probiotics have emerged as promising agents for managing skin aging. However, maintaining probiotic viability in topical formulations is a key challenge. Immobilizing probiotics in natural carriers such as kombucha-derived bacterial cellulose (KBC) offers a potential solution for enhancing stability and efficacy.

Aims & Objectives: This study aimed to develop a stable topical gel formulation containing *Lactobacillus* spp. Immobilized within KBC and to evaluate its anti-aging potential, particularly against UV-induced photoaging in a murine model.

Methods: KBC was prepared by fermenting butterfly pea flower-infused tea using a symbiotic culture of bacteria and yeast (SCOBY), followed by purification, drying, and milling. *Lactobacillus* strains were cultured from curd and confirmed using biochemical assays. The bacteria were immobilized onto KBC powder that was incorporated into a gel and evaluated for pH and spreadability. A photoaging model using C57BL/6J mice was standardized through UV-A exposure and topical MSA treatment. The anti-aging effect of the formulation was assessed by measuring wrinkle reduction, collagen and elastin levels, antioxidant status, and inflammatory mediators.

Results: The efficiency of immobilized bacteria onto KBC was 69.4% and viable cell count of 1.25×10^5 CFU/g was achieved. The gel formulation showed appropriate physicochemical characteristics and demonstrated significant preventive effects against photoaging in mice. Treated groups exhibited reduced wrinkle formation, improved collagen and elastin content, enhanced antioxidant activity, and decreased inflammation.

Conclusion: The KBC-based probiotic gel presents a promising natural and biocompatible approach for preventing photoaging, with potential applications in advanced dermatological care and skincare therapeutics.

Keywords: Anti-aging, Skin, *Lactobacilli*, KBC (Kombucha Biocellulose).



PHA-BT-028: Evaluation of the Dietary Fibers of Chia Seeds in Alleviating Depression Associated with Type 2 Diabetes in Rats

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Background: Type 2 diabetes mellitus (T2DM) is a chronic metabolic disorder frequently associated with depression, primarily due to dysregulation of the gut–brain axis and gut microbiota imbalance, where impaired intestinal barrier function promotes microbial translocation and systemic inflammation, subsequently leading to oxidative stress and neurotransmitter disturbances, particularly involving dopamine. Glucagon-like peptide-1 (GLP-1), an incretin hormone, plays a key role in glucose regulation, neuroprotection, and gut-brain signaling. Dietary fibers from chia seeds (*Salvia hispanica* L.) Are rich in soluble components like mucilage and polysaccharides, which are known to modulate gut microbiota, enhance GLP-1 secretion, and improve metabolic and behavioral outcomes.

Aims & Objectives: This study aimed to extract and characterize dietary fibers from chia seeds and to evaluate their antidepressant potential in a rat model of T2DM-induced depression, focusing on modulation of the gut–brain axis through microbiota regulation.

Methods: In this study, dietary fibers were extracted from chia seeds (*Salvia hispanica* L.), and characterized for swelling index, water/oil holding capacity, viscosity, and FTIR spectral properties. T2DM was induced in Wistar rats using a high-fat diet followed by streptozotocin (25 mg/kg, i.p.). Depressive-like behaviors were assessed through tail suspension, Cook's pole climbing, and actophotometer tests. Intestinal permeability was evaluated by phenol red and lactulose–mannitol assays. Biochemical analysis encompassed oral glucose tolerance test (OGTT), inflammatory markers (TNF- α , IL-10), dopamine level, GLP-1 levels and oxidative stress markers (GSH, catalase, SOD).

Results: Chia seeds dietary fiber significantly improved behavioral responses, reduced inflammatory cytokines and intestinal permeability, elevated GLP-1 and dopamine levels, and restored antioxidant status.

Conclusion: These findings suggest that chia seed dietary fibers exert therapeutic effects against T2DM-associated depression via modulation of the gut-brain axis, highlighting their potential as a natural dietary intervention.

Keywords: Chia seeds, Dietary fiber, Type 2 Diabetes Mellitus, Depression, GLP-1, Gut-brain axis



PHA-BT-029: Development of RP-HPLC method for simultaneous determination of dapagliflozin and sitagliptin in rat plasma: method validation and application in pharmacokinetic studies

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Aims & Objectives: To develop a new, straightforward, accurate, and precise simultaneous estimation of dapagliflozin and sitagliptin by RP-HPLC in rat plasma and validate the developed method as per ICH guidelines. To evaluate In vivo Pharmacokinetic parameters for Dapagliflozin and Sitagliptin by RP-HPLC in rat plasma.

Methods: A mobile phase of 40:60% v/v of acetonitrile and water at pH 7.0 was used for chromatographic separation. The Phenomenex Luna C 18 column (250 x 4.6 mm, 5 µm particle size) was utilized, and it was set to run at a rate of 1.2 ml/min utilizing PDA detection at 210 nm.

Results: Sitagliptin and dapagliflozin had retention times of 5.6 and 6.6 minutes, respectively. It was discovered that the approach outlined was linear for both dapagliflozin (50–250 ng/ml) and sitagliptin (500–2500 ng/ml). For dapagliflozin and sitagliptin, the correlation coefficients were determined to be 0.9994 and 0.9997, respectively. Dapagliflozin was found to have limits of quantification (LOQ) and detection (LOD) of 10.81572 ng/ml and 3.569 ng/ml, respectively, whereas sitagliptin was found to have limits of 84.47158 and 27.87562 ng/ml.

Conclusion: The outcomes show that the bio-analytical approach is linear, accurate, and exact. After validation, the devised approach was deemed appropriate for use in the design of pharmacokinetic investigations using a simple solvent system.

Keywords: Dapagliflozin, Sitagliptin, RP-HPLC, Bioanalytical method, Pharmacokinetics.



PHA-BT-030: Identification of key target using geo2r and plant-derived ligands for the therapeutic application of endometriosis in female wistar rats

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Introduction: This study focusing on genomic-level identification of key targets for therapeutic intervention. It highlights prostacyclin synthase (PTGIS) as a promising target. The research aims to evaluate Baicalein, identified as an antagonist to PTGIS, for its anti-proliferative, anti-angiogenic, and anti-platelet effects, with the potential to develop novel plant-based therapies.

Aim:

- To analyze differentially expressed genes (DEG) in endometriosis using GEO2R to identify a significant target.
- To evaluate the binding affinity of selected phytoconstituents, specifically Baicalein, with the chosen target (PTGIS) through in silico molecular docking, MM-GBSA, and molecular dynamics.
- To evaluate the in-vivo antiproliferative activity of the selected phytoconstituent against surgically induced endometriosis in female Wistar rats.

Methods:

The methodology employed in this study involved a multi-pronged approach:

1. DEG analysis: Differentially expressed genes (DEG's) in Endometriosis were screened using GEO2R analysis.
2. In-silico methods: These included molecular docking and ligand interaction studies to assess the binding affinity of potential compounds.
3. In-vivo studies: Endometriosis was surgically induced in female Wistar rats to establish an animal model for evaluating therapeutic efficacy.

Results: PTGIS was identified as a key target, appearing among the top 5 upregulated genes with a Log Fc of 3.843 and an Adj.P.value of 0.00119. In silico molecular docking results demonstrated that Baicalein achieved a docking score of -10.906 and an MMGBSA score of -45.08.

Conclusion: This study successfully identified (PTGIS) as a promising therapeutic target for endometriosis. Baicalein, a phytoconstituent, was recognized as a potential antagonist to PTGIS, showing encouraging binding affinities in in-silico evaluations.



PHA-BT-031: Metagenomic Insights into Gut Microbiome Dysbiosis and Metabolic Pathway Alterations in Obesity

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Background: Obesity, impacting over 650 million individuals globally, is intricately associated with gut microbiota dysbiosis. This microbial imbalance contributes to metabolic dysfunction by altering energy extraction from food, modulating short-chain fatty acid production, and compromising gut epithelial integrity. Advancements in metagenomic and metabolomic technologies have enabled a shift from descriptive microbial studies to mechanistic investigations aimed at elucidating microbial contributions to obesity.

Aims & Objectives: To investigate the compositional and functional differences in the gut microbiome between obese and lean individuals, and to identify microbial taxa and metabolic pathways significantly associated with obesity.

Methods: Shotgun metagenomic sequencing was conducted on fecal samples collected from 100 obese (BMI ≥ 30) and 100 lean (BMI ≤ 25) participants. Taxonomic composition was profiled using metaphlan4, and metabolic pathways were analyzed using humann3. Statistical associations were assessed via maaslin2.

Results: A notable increase in the Firmicutes/Bacteroidetes ratio was observed in obese subjects (3.2 vs. 1.1 in lean), alongside significant upregulation of lipid biosynthesis pathways (log2 fold change = 2.3). Notably, the abundance of *Akkermansia muciniphila* demonstrated a strong inverse correlation with BMI ($r = -0.67$).

Conclusion: Distinct microbial and metabolic signatures associated with obesity were identified, underscoring the potential of targeting the gut microbiome through probiotics or dietary interventions as a therapeutic strategy for metabolic disorders.

Keywords: Gut microbiome, Obesity, metaphlan4, humann3, Firmicutes, *Akkermansia muciniphila*.



PHA-BT-032: Combating Glucose Cataract with Repurposed Drugs: A Biofilm Delivery Study Using Goat Eye Lens

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Background: Cataract remains a major cause of visual impairment, with glucose-induced lens opacity being a common manifestation in diabetic conditions. Conventional treatments are invasive and limited in accessibility. This study proposes a novel, non-invasive drug delivery strategy using repurposed drug-coated ocular biofilms. The goat eye lens is used due to its anatomical and physiological similarity to the human lens which was employed as an ex-vivo model to evaluate the formulation's efficacy.

Aims & Objectives: To evaluate the efficacy of drug-loaded ocular biofilm in preventing glucose-induced cataract. Key objectives included formulation of biofilm, confirmation of drug content, induction of cataract, and assessment of physicochemical and biochemical outcomes.

Methods: Melatonin and α -lipoic acid were incorporated into chitosan-HPMC-based biofilms using the solvent casting technique. Molecular docking was conducted using Auto Dock software to evaluate the binding affinity of both compounds with various targeting site. FTIR confirmed drug-polymer compatibility. Cataract was induced by incubating goat eye lenses in 55 mM glucose, followed by treatment with formulated biofilms. Lens opacity was assessed visually over 72 hours. Biochemical parameters analysed included total protein, SOD, CAT, GSH, and MDA.

Results: The optimized film (FT5) exhibited uniformity and 96% drug content. In-vitro drug release showed a sustained profile with cumulative release of 52.2% for melatonin and 53.9% for α -lipoic acid at 240 minutes. Group V (melatonin + α -lipoic acid) preserved maximum lens transparency compared to control and individual drug groups. Biochemical assays confirmed significantly improved antioxidant activity and reduced oxidative stress markers in Group V.

Conclusion: The combination of melatonin and α -lipoic acid in a biofilm delivery system showed strong therapeutic efficacy in delaying glucose-induced cataract. This non-invasive approach demonstrated promising antioxidant potential and lens protection, suggesting its viability as an alternative to conventional cataract management strategies.

Keywords: Drug repurposing, glucose induced cataract, ocular biofilm, Melatonin, α -Lipoic acid, goat lens model.



PHA-BT-033: Culinary herbs derived essential oils for management of Non-alcoholic fatty liver disease; A preliminary *In-vitro* study

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Background: Non-alcoholic fatty liver disease (NAFLD) is a global health concern lacking effective pharmacotherapy. *In-vitro* models, particularly palmitic-oleic acid (POA) induced hepg2 cell model, are vital for understanding NAFLD pathogenesis and screening therapeutic candidates. Culinary herbs, rich in bioactive compounds, offer potential for managing metabolic disorders.

Aim & Objective: To elucidate the beneficial role of culinary herbs derived essential oil against palmitic acid and oleic acid (POA) induce fat accumulation and insulin resistance in hepg2 Cell line.

Methodology: hepg2 cells were exposed to a physiological ratio of POA to induce steatosis including intracellular fat accumulation and cellular stress. Cells were co-treated with various concentrations of different essential oil which was selected on the basis of literature survey. Intracellular lipid accumulation was quantified by Oil Red O staining and Glucose uptake through GOD-POD method indicating insulin sensitivity. Cell viability was monitored throughout the experiments.

Results: Exposure of POA is able to induce fat accumulation and insulin resistance in hepg2 cell line, human liver cancer cell line. Preliminary findings demonstrate that out of four essential oil one showed significant ($P < 0.05$) inhibition in fat accumulation and improved glucose uptake when compared to vehicle treated hepg2 cell indicating their anti- steatotic properties.

Conclusion: This *in-vitro* screening provides valuable insights into the potential of culinary herbs as natural interventions for NAFLD. Identifying specific herbs with strong anti-steatotic and insulin-sensitizing properties can pave the way for further investigation and development of novel dietary strategies or phytomedicines for NAFLD management.

Keywords: NAFLD, hepg2, fat accumulation, Insulin resistance, culinary herbs.



PHA-BT-034: Evaluation of Complex Interaction of Circadian Rhythm and Gut Microbiota to Enhance the Effect of 5-Fluorouracil on DMH Induced Colon Cancer in Rats

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Background: Colon cancer remains a leading cause of global cancer mortality. Recent evidence suggests that circadian rhythm and gut microbiota significantly influence cancer progression and therapeutic outcomes. Aligning drug administration with the body's internal clock termed chronotherapy could enhance drug efficacy while minimizing toxicity. Additionally, gut microbiota modulation is emerging as a novel adjuvant strategy in cancer therapy.

Aims & Objectives: To investigate the synergistic effect of circadian-timed 5-Fluorouracil (5-FU) administration and gut microbiota modulation on DMH-induced colon cancer in rats.

Methods: Sprague- Dawley rats were divided into 7 groups: normal control, disease control (DMH 20 mg/kg, i.p. Once weekly for 12 weeks), and four treatment groups receiving 5-FU (33 mg/kg, i.p.) At 2 AM, with or without probiotic supplementation (Lactobacillus and Bifidobacterium, 2 billion CFU/day orally). Probiotic treatment commenced two weeks before DMH administration and continued throughout the study. Post-treatment, tumor weight, tumor burden, number of aberrant crypt foci (ACF), histopathology, and organ indices were assessed.

Results: The study showed significant reduction in tumor weight, burden, and aberrant crypt foci in rats treated with 5-FU at 2 AM, especially when combined with folic acid or gut microbiota. Histopathology confirmed improved colonic architecture. Chronotherapy and adjuvant modulation enhanced 5-FU's anticancer efficacy with reduced toxicity.

Conclusion: Chronotherapy and adjuvant therapy with folic acid or gut microbiota significantly enhanced 5-FU's anticancer activity. Among all groups, Group 5 (5-FU + folic acid at 2 AM) showed the most effective reduction in tumor burden and ACF. Timed administration optimized efficacy and minimized toxicity.

Keywords: Chronotherapy, 5-Fluorouracil, Gut Microbiota, Circadian Rhythm, Colon Cancer, DMH



PHA-BT-035: Nature's Arsenal: Targeting MCF-7 Breast Cancer Cells with *Elaeocarpus sphaericus* and *Cordyceps militaris* Extract

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Breast cancer is still the biggest cause of cancer-related mortality in the globe, with both incidence and fatality rates increasing dramatically. Despite advances in therapeutic approaches, oestrogen receptor-positive (ER+) breast cancer subtypes, such as MCF-7, provide considerable treatment problems due to their aggressive nature and proclivity for therapy resistance. In this study, we evaluated the combined anticancer effects of *Elaeocarpus sphaericus* (ESM) and *Cordyceps militaris* aqueous extract (ACE) on MCF-7 breast cancer cells. The MTT experiment verified that the combined treatment had a potent IC₅₀ value of 36.01 ± 0.05 $\mu\text{g/ml}$, exceeding the reference medication, doxorubicin (IC₅₀: 58.19 ± 0.05 $\mu\text{g/ml}$). Apoptosis examination with Annexin V/PI labelling revealed a considerable increase (68.72%) in apoptotic cell populations compared to the control group. Cell cycle research revealed G2/M and Sub G0/G1 phase arrest, which successfully stopped cancer cell proliferation. Furthermore, the wound healing assay verified the combination's anti-metastatic effects, with wound closure at 10.11% after 48 hrs against 48.80% in untreated cells. Our findings indicate that the combined ESM and ACE extracts have a multi-targeted effect, boosting apoptosis, causing cell cycle arrest, and reducing metastasis, providing a novel and potential therapeutic method for breast cancer treatment. This discovery provides the path for future molecular research to explain the precise processes driving these synergistic effects, as well as the creation of anticancer therapies based on plants and fungi.

Keywords: Breast cancer, *Elaeocarpus sphaericus*, *Cordyceps militaris*, Apoptosis, cell cycle analysis



PHA-BT-036: Neuroprotective Effects of Mangiferin Against Methotrexate and 5-Fluorouracil-Induced Cytotoxicity in C6 Glioma Cells: An In Vitro Study)

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Background: Chemotherapy-induced cognitive impairment (CICI), commonly referred to as “chemo brain,” is a debilitating side effect observed in cancer survivors receiving agents like Methotrexate (MTX) and 5-Fluorouracil (5-FU). These drugs exert neurotoxicity through apoptosis, oxidative stress, and glial cell activation. Mangiferin, a xanthone glucoside derived from *Mangifera indica*, has demonstrated potent antioxidant and neuroprotective activity.

Aims & Objectives: To evaluate the neuroprotective effect of Mangiferin against MTX+5-FU-induced cytotoxicity in C6 rat glial cells and to assess its ability to prevent apoptosis and improve cell survival.

Methods: C6 glial cells were exposed to MTX+5-FU combination (1:1) to determine IC₅₀, followed by pretreatment with Mangiferin at non-toxic concentrations (80 µm and 100 µm). Cell viability was measured using the Sulforhodamine B (SRB) assay, while apoptosis was assessed by Acridine Orange/Ethidium Bromide (AO/EB) staining.

Results: MTX+5-FU significantly reduced C6 cell viability (~46–30%) and increased apoptosis (~18–22%). Mangiferin pretreatment restored cell viability to ~74% and reduced apoptosis to ~1–2.6%, indicating dose-dependent neuroprotection.

Conclusion: Mangiferin exhibits significant neuroprotective potential against MTX+5-FU-induced cytotoxicity in glial cells. These findings support its possible role as an adjuvant therapy to prevent chemotherapy-associated neurotoxicity.

Keywords: Mangiferin, Chemobrain, C6 glioma cells, Neuroprotection, Methotrexate, 5-Fluorouracil, Apoptosis, SRB assay



PHA-BT-037: Fruit Waste to Pharma Treasure: Anticancer Potential of *Carica papaya* (Papaya) Peel Phytochemicals

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Background: *Carica papaya* (Papaya), a tropical fruit, is highly valued in traditional medicine for its therapeutic properties, but its bioactive potential in its fruit peel remains largely unexplored.

Aims & Objectives: This study set out to characterize the phytochemical makeup of ethanolic *C. Papaya* peel extract and to assess its anticancer potential through both computational modelling and cell-based assays.

Methods: The peel extract's key phytoconstituents, including myo-inositol, were identified through high-resolution Q-TOF LC-MS profiling. The extract's cytotoxic effects on MCF 7 proteins were evaluated using MTT assay, complemented by light microscopy, and the most abundant compound was docked against inhibitor of apoptosis proteins.

Results: LC-MS analysis revealed a spectrum of phenolic and inositol derivatives, with myo-inositol predominating among identified components. *In silico* docking indicated a robust and favorable interaction between myo-inositol and apoptosis regulating protein targets. *In vitro*, the peel extract induced pronounced, dose-dependent cytotoxicity in MCF 7 cells, accompanied by hallmark apoptotic changes such as cell shrinkage, membrane blebbing, detachment and altered cell morphology.

Conclusion: Ethanolic extract of *C. Papaya* fruit peel harbors bioactive phytochemicals, most notably myo-inositol, that exhibit promising anticancer activity both virtually and in cultured breast cancer cells. These findings support further exploration of papaya peel as a rich source of natural compounds for cancer therapeutics.

Keywords: *Carica papaya*, myo-inositol, anticancer.



PHA-BT-038: High Pressure Homogenized Cucurbitacin B Nanosuspension for targeting Rheumatoid Arthritis: Characterization and In Vitro–In Vivo Correlation.

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Background: Cucurbitacin B is a powerful anticancer triterpenoid constrained by significantly low water solubility and limited oral bioavailability. Nanosuspension technology can significantly improve dissolution and permit predictive in vitro–in vivo correlations (IVIVC).

Aims & Objectives: To develop a high-pressure-homogenized Cucurbitacin B nanosuspension; to characterize its particle size, polydispersity index (PDI), zeta potential, entrapment efficiency and morphology; to assess in vitro release kinetics; and to establish Level A IVIVC.

Methods: Nanosuspensions were created through high pressure homogenization (500–1700 bar; 20 cycles). Mean particle size and PDI were measured using dynamic light scattering; zeta potential was determined through laser Doppler electrophoresis; ultrafiltration HPLC quantified entrapment efficiency; SEM was used to examine morphology. Release studies were performed in pH 1.2 and pH 6.8 environments (USP II), and the release data were analyzed using kinetic models. IVIVC was established employing deconvolution (Wagner–Nelson) based on available rat pharmacokinetic data.

Results: The optimized formulation achieved a mean particle size of 426.3 ± 5.8 nm, PDI 0.543 ± 0.01 , and zeta potential -34.2 ± 1.0 mV. SEM revealed spherical nanoparticles. Over 80% of drug was released within 20–30 min in both media. Level A IVIVC exhibited $R^2 = 0.96$ with prediction errors $<10\%$ for C_{max} and AUC.

Conclusion: The Cucurbitacin B nanosuspension, processed through high pressure homogenization, demonstrated significantly enhanced dissolution kinetics and attained a robust Level A in vitro–in vivo correlation, allowing precise forecasting of its in vivo pharmacokinetic behavior.

Keywords: Cucurbitacin B, Nanosuspension, High-pressure homogenization, *in vitro* release kinetics, IVIVC



PHA-BT-039: Repurposing Bilastine for Atopic Dermatitis: A Dual-Action Preclinical Study

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Atopic dermatitis (AD) is a chronic, relapsing skin disorder. It involves epidermal barrier dysfunction, immune imbalance, and oxidative stress (OS). Current treatments rely heavily on corticosteroids (CS), which offer short-term relief but cause side effects with long-term use. This highlights the need for safer, steroid-sparing alternatives. Bilastine (BL) is a second-generation H₁-antihistamine with high receptor selectivity and limited central nervous system (CNS) penetration. While approved for allergic conditions, its role in AD remains underexplored. This study addresses that gap by evaluating the therapeutic effects of BL in a 2,4-dinitrochlorobenzene (DNCB)-induced rat model of AD. BL was administered both orally and topically for 16 days. Treated groups showed visible improvement in skin symptoms such as erythema, edema, and thickening. Biochemical assays indicated reduced levels of pro-inflammatory cytokines including tumor necrosis factor-alpha (TNF-α), interleukin-6 (IL-6), interferon-gamma (IFN-γ), and cyclooxygenase-2 (COX-2). Markers of OS also improved, with lowered reactive oxygen species (ROS), lipid peroxidation (LPO), and hydroperoxides (hpx). Antioxidant enzymes like catalase (CAT), superoxide dismutase (SOD), and glutathione S-transferase (GST) were restored toward normal levels. Histological analysis showed reduced eosinophil and mast cell infiltration. *In silico* docking revealed strong binding of BL to COX-2, glutathione (GSH), and GST, suggesting multi-target activity. This study addresses a significant research gap by demonstrating the dual anti-inflammatory and antioxidant properties of BL in AD. The findings support its repositioning as a potential steroid-free therapeutic agent. Further clinical research is warranted to explore its role in human AD management.

Keywords: 2,4-Dinitrochlorobenzene (DNCB) model, mast cell degranulation, T-helper 2 immune response, molecular docking, Histamine 1-antihistamine, antioxidant, anti-inflammatory.



PHA-BT-040: Analysis of significant targets using GEO2R and Exploration of Phytoconstituents for Possible Therapeutic Benefits in Multiple Sclerosis

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AIM: The aim of the study is to identify significant targets in MS through analysis of DEG using GEO2R and selection of suitable phytoconstituent through computational models.

OBJECTIVES:

- To analyze differentially expressed genes (degs) in multiple sclerosis using GEO2R and identify a significant target.
- To evaluate the binding affinity and stability of the selected phytoconstituent with chosen target through in silico molecular docking, MM-GBSA and molecular dynamics.
- To assess the beneficial effect of selected phytoconstituent in rat model of multiple sclerosis.
- To estimate the level of antioxidants, GSH, Catalase, SOD, LPO.
- To assess histopathological changes in the corpus callosum region using Hematoxylin and Eosin staining.
- Estimation of TNF- α

Methods: The study follows a three-phase methodology: (1) Identification of key molecular targets using GEO2R to analyze differentially expressed genes (degs) in MS. (2) In Silico Screening of Phytoconstituents through molecular docking, MMGBSA, and molecular dynamics using Schrodinger Suite 2022-4 to identify potential therapeutic compounds. (3) Preclinical In Vivo Evaluation using a Cuprizone-induced (400 mg/kg, p.o.) MS model, followed by behavioral assessments and antioxidant analysis to validate neuroprotective effects.

Results: Following the analysis of differentially expressed genes (degs) in multiple sclerosis using GEO2R, TACE was selected as the target gene due to its potential role in promoting inflammation and disease progression, making it a promising candidate for therapeutic intervention. Preliminary in-silico screening identified Diosmetin as having the highest binding affinity to the selected target, with a docking score of -10.02 kcal/mol and an MMGBSA score of -101.19 kcal/mol. The in vivo study aims to show decreased inflammation, oxidative damage, and enhanced remyelination, confirming its potential as an effective therapeutic approach.

Conclusion: This investigation seeks to confirm TACE's role as a viable therapeutic target in treating Multiple Sclerosis, while also discovering naturally-occurring compounds that can effectively modulate its activity. By generating strong preclinical evidence, it seeks to pave the way for safer, cost-effective treatment options.

Abbreviations: Multiple Sclerosis, differentially expressed genes



PHA-BT-041: Genome Mining for Surfactin Production in *Bacillus subtilis* Strains

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Background:

Surfactin, a potent biosurfactant produced by *Bacillus subtilis*, exhibits broad-spectrum antimicrobial activity and industrial relevance. However, variations in surfactin biosynthesis among *B. Subtilis* strains hinder consistent large-scale production. Understanding genetic diversity in biosynthetic gene clusters (bgcs) is critical to optimizing yield.

Aim & Objectives:

To identify and compare surfactin biosynthetic gene clusters (bgcs) across multiple *B. Subtilis* strains and correlate genetic architecture with surfactin yield.

Methods:

Surfactin bgcs were predicted using antismash and PRISM platforms. Comparative genomic analyses of the strains were performed using orthofinder and Mauve alignment tools. High-performance liquid chromatography (HPLC) quantified surfactin levels.

Results:

Strain ATCC 21332 exhibited a 25% larger *srfa* operon compared to NCIB 3610, aligning with a twofold increase in surfactin production (1.8 g/L vs. 0.9 g/L). This suggests operon length and structure significantly influence yield.

Conclusion:

Genomic insights into the *srfa* operon can guide metabolic engineering strategies to enhance surfactin biosynthesis, facilitating its application in pharmaceuticals and environmental biotechnology.

Keywords: Surfactin, *Bacillus subtilis*, antismash, biosynthetic gene clusters, *srfa* operon

PHA-BT-042: Probiotics-Induced Restoration of Glycocalyx for Colitis Treatment

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Background:

Ulcerative colitis (UC), a major subtype of inflammatory bowel disease (IBD), is characterized by persistent inflammation of the colonic mucosa, epithelial barrier disruption, and gut dysbiosis. The hallmark of UC is the depletion of the glycocalyx, a mucin-rich layer vital for microbial homeostasis and epithelial protection. Conventional therapies offer limited potential to restore this structure. Probiotics have emerged as promising agents for gut microbiota modulation and mucosal repair. Kombucha-derived bacterial cellulose (KBC) provides a biocompatible, porous scaffold to immobilize probiotics and enable colon-targeted delivery.

Aims & Objectives: To develop a KBC-based colon-targeted probiotic formulation and evaluate its efficacy in glycocalyx restoration and colitis symptom alleviation in a murine model.

Methods: KBC was obtained by fermenting butterfly pea flower tea with SCOBY, followed by purification, drying, and milling. Lactobacillus strains were isolated from curd, identified, and immobilized onto KBC powder. The formulation was suspended in a colon-targeting polymer and subjected to *In vitro* release studies under pH-specific conditions. BALB/c mice were administered antibiotics for 10 days to induce dysbiosis, followed by 2.5% DSS for 4 days to induce colitis. Mice were treated with probiotic-KBC formulation for 14 days. Parameters evaluated included Disease Activity Index (DAI), colon length and morphology, antioxidant levels (SOD, catalase, GSH), serum cytokines (TNF- α , IL-10), histopathology, and glycocalyx assessment using lectin binding. SEM confirmed uniform microparticle size ($\sim 12.4 \mu\text{m}$).

Results: Treatment improved DAI, antioxidant status, cytokine balance, and histological features. Notably, glycocalyx restoration was evident in treated groups, confirming effective colon targeting and mucosal healing.

Conclusion: The probiotic-KBC system offers a natural scaffold-based approach for targeted probiotic delivery and glycocalyx regeneration, representing a novel strategy for UC therapy.

Keywords: Ulcerative colitis, Glycocalyx restoration, Kombucha bacterial cellulose (KBC).



PHA-BT-043: Evaluation for bone mineralization and bone strength of *Limonia acidissima* Nanosuspension effects in Dexamethasone-induced Osteoporosis in rats

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Background: *Limonia acidissima* (wood apple) is traditionally used for bone health due to its high calcium, phosphorus, vitamins D, C, and K content. However, no animal studies support its anti-osteoporotic potential. This study aimed to develop an oral nanosuspension of *L. Acidissima* to enhance bioavailability, solubility, site-specific action, and therapeutic efficacy against dexamethasone-induced osteoporosis in rats.

Methodology: Network pharmacology (Cytoscape 3.7.2) and molecular docking (Schrödinger) were employed to identify active pathways and targets. Osteoporosis was induced in rats using dexamethasone (7 mg/kg), followed by treatment with alendronate (standard) and *L. Acidissima* nanosuspension (200, 400, 800 mg/kg p.o.) For 35 days. Parameters such as body weight, bone length, diameter, hardness, and biochemical markers (serum calcium, phosphorus, urine calcium/phosphorus, SOD, GSH, ALP, TNF- α , IL-1 β) were assessed.

Results: LC-MS analysis of the extract identified stigmasterol, β -sitosterol, and riboflavin as key compounds. In silico analysis showed modulation of PI3K-Akt, AMPK, and estrogenic signaling pathways, enhancing osteoblast activity and calcium homeostasis. Nanosuspension was optimized using a 3² factorial design and characterized by particle size, viscosity, and SEM. Dexamethasone reduced body weight and bone biomarkers, while LANS (400 mg/kg and 800 mg/kg) reversed these changes, improving mineralization and inflammatory status.

Conclusion: *L. Acidissima* nanosuspension demonstrated superior anti-osteoporotic activity over the extract alone, likely due to improved bioavailability. Its phytoconstituents target bone remodeling, reduce inflammation, and promote bone strength, suggesting potential as a therapeutic agent for osteoporosis

Key words- Nanosuspension *Limonia acidissima*, osteoporosis, dexamethasone, Stigmasterol, AMPK, P13-Akt, tnfa, IL-1 β .



PHA-BT-044: Integrative Approach of Computational Modelling and Pharmacological Studies to Develop Novel Therapeutics for Management of Myocardial Infarction

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Background:

Myocardial infarction (MI) remains a leading cause of mortality worldwide. Despite advancements in pharmacotherapy, novel therapeutic strategies are essential for effective management. Nattokinase, a fibrinolytic enzyme, has shown promise in cardiovascular health due to its antithrombotic and cardioprotective potential.

Aims & Objectives: This study aims to investigate the cardioprotective potential of a test formulation based on Nattokinase through an integrative approach involving computational modelling and pharmacological evaluation.

Methods:

In-silico molecular docking was conducted to predict the interaction of Nattokinase with key cardiovascular targets, including TNF- α , IL-6, and PPAR- γ . A stable formulation of Nattokinase was developed and characterized. Sub-acute toxicity was evaluated following OECD guideline 407 using Albino Wistar rats. Cardioprotective efficacy was studied in two MI models: Olanzapine-induced and high-fat diet-induced myocardial infarction in rats. Parameters assessed included ECG, serum biomarkers (CK-MB, LDH, troponin), oxidative stress markers, and histopathological analysis.

Results:

Molecular docking indicated strong binding affinities of Nattokinase with inflammatory and metabolic targets. The developed formulation demonstrated stability and safety in sub-acute toxicity studies. In both MI models, the test formulation significantly ameliorated myocardial injury, improved ECG profiles, reduced oxidative stress, and restored histoarchitecture compared to control.

Conclusion:

The integrative approach combining in-silico modelling and pharmacological evaluation substantiates the therapeutic potential of Nattokinase in myocardial infarction. This study supports further translational development of Nattokinase-based therapies for cardiovascular diseases.

Keywords:

Myocardial infarction, Nattokinase, In-silico docking, Cardioprotection, Oxidative stress, Olanzapine, High-fat diet



PHA-BT-045: Rational Design and Evaluation of a Modified HVEM-Derived Peptide as a Novel Entry Inhibitor Against Herpes Simplex Virus Type 1

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Background: Herpes simplex virus type 1 (HSV-1) remains a significant global health concern, with current antiviral therapies facing challenges such as drug resistance and limited curative potential. Peptide-based therapeutics offer promising alternatives due to their specificity and reduced side effects. This study focuses on the rational design, optimization, and evaluation of a modified peptide derived from the herpesvirus entry mediator (HVEM), targeting the critical gd-HVEM interaction essential for HSV-1 entry.

Objective: To enhance the therapeutic efficacy and stability of an HVEM-derived peptide for effective inhibition of HSV-1 entry, through in silico modifications and in vitro validation.

Methodology: In this study, we employed a combination of computational and experimental approaches to design and evaluate an HVEM-derived peptide as an entry inhibitor against HSV-1. Residue scanning was performed to identify key positions for mutation, leading to the rational design of seven peptide variants. Their three-dimensional structures were predicted using PEPFOLD3, and physicochemical properties such as solubility and charge were assessed with expasy-protparam. Protein-peptide docking (clustpro) and MM-GBSA calculations were conducted to prioritize variants with improved binding to HSV-1 glycoprotein D. The top candidates underwent molecular dynamics simulations to assess complex stability. The most promising peptide was synthesized, and its antiviral activity was evaluated in vitro using cytopathic effect (CPE) inhibition and TCID50 assays in Vero cells.

Result & Conclusion: Residue scanning and modeling identified several HVEM-derived peptide variants with enhanced physicochemical properties and predicted stability. Docking and binding energy calculations highlighted one variant (F4P3) with superior affinity for HSV-1 glycoprotein D, and molecular dynamics simulations confirmed its stable binding. The synthesized peptide demonstrated high solubility and no cytotoxicity up to 250 µg/ml. In vitro assays showed up to 59% protection against HSV-1 at 150 µm and a significant reduction in viral replication. These findings establish the optimized HVEM-derived peptide as a promising novel entry inhibitor, supporting its potential for further development as an alternative or adjunct antiviral therapeutic against HSV-1.



PHA-BT-046: Evaluation of donepezil-aroma combination for mitigating dementia in Amyloid beta (1-42) induced mice model for Alzheimer's disease

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Background: Early olfactory dysfunction affects over 80% of Alzheimer's disease (AD) patients, hinting at the olfactory system's role in disease progression. Essential oils like lavender and coriander have shown promise in neuroprotection. This study investigates olfactory-directed therapy in AD using a novel donepezil-aroma combination.

Aims & Objectives: To assess olfactory involvement in AD pathology and evaluate the therapeutic potential of lavender and coriander oil inhalation, both individually and in combination with donepezil, for reversing cognitive and neuronal deficits in an A β 1-42-induced mouse model.

Methods: Female C57BL/6 mice were chronically exposed to cigarette smoke to induce olfactory impairment. AD was modeled using intracerebroventricular A β 1-42 injection. Behavioral assays and neurochemical analyses examined olfaction and cognition. GC/MS-analyzed oils were nebulized and administered post-injection, followed by oral donepezil. Neurodegeneration and AD-relevant protein expression were quantified via western blot in hippocampal and bulbar tissues.

Results: A β 1-42 and smoke exposure caused significant olfactory and cognitive dysfunction, elevated hippocampal glutamate, and decreased neuronal viability. Inhalation of diluted essential oils improved memory performance and neurotransmitter balance. The donepezil-lavender combination demonstrated superior efficacy, reversing memory impairment, reducing A β and phosphorylated tau, and restoring neuronal integrity. Olfactory marker expression in the bulb supported tissue-level recovery.

Conclusion: Olfactory system damage is a critical element in AD pathology. This study highlights a promising therapeutic angle targeting olfaction with essential oils and donepezil to reverse dementia-like symptoms and promote neural regeneration.

Keywords: Alzheimer's Disease, Olfactory Dysfunction, A β 1-42, Donepezil, Lavender Oil, Neuroprotection



PHA-BT-047: Evolutionary Dynamics and Positive Selection of CYP3A Genes in Insecticide-Resistant *Blattella germanica*

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Background:

Blattella germanica (German cockroach) poses significant public health threats, particularly in urban settings, due to its role in allergen production and disease transmission. A major obstacle in its control is the rapid development of resistance to pyrethroid insecticides, largely attributed to the overexpression and mutation of the cytochrome P450 CYP3A genes.

Aims & Objectives: This study aims to investigate the evolutionary dynamics of the CYP3A gene family in *B. Germanica* and to identify genetic adaptations—such as mutations, gene duplications, and positively selected sites—that contribute to insecticide resistance. It also evaluates the impact of various insecticide deployment strategies on resistance evolution.

Methods: Gene sequences were obtained from both public databases (NCBI, vectorbase) and field-collected resistant and susceptible strains. MAFFT v7 was used for codon-based alignment. Phylogenetic relationships were assessed using raxml with the GTR+G model and 1000 bootstrap replicates. Positive selection was tested using PAML (M8 vs M8a models), and gene duplications were identified through synteny and read-depth analyses. Structural implications of mutations were explored via homology modeling.

Results: Phylogenetic analysis segregated CYP3A variants into distinct clades, with resistant strains forming a separate lineage. The G137D mutation was significantly associated with resistance ($p = 0.003$). PAML analysis identified four codon sites under positive selection, particularly near the heme-binding domain. Gene duplication events were observed in resistant strains, correlating with increased copy number and detoxification capacity. Structural modeling suggested altered pyrethroid binding efficiency due to key mutations.

Conclusion: Insecticide pressure has driven adaptive evolution in the CYP3A gene family of *B. Germanica*, including point mutations and gene duplications that enhance detoxification. These findings underscore the necessity of adopting integrated pest management strategies and support the potential of CYP3A inhibition as a novel target in resistance mitigation.

Keywords: CYP3A, *Blattella germanica*, Insecticide resistance, Gene duplication, Positive selection, PAML, Phylogenetics



PHA-BT-048: Green Synthesis of Zinc Oxide Nanoparticles using *Martynia annua* Leaf extract: Characterization, Evaluation of Antidiabetic, and Anti-Nephropathy Potentials in Rat Model

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Background: *Martynia annua*, commonly known as Kakanasika, is an annual herb well-known for its diverse medicinal properties, including analgesic, antipyretic, antibacterial, anticonvulsant, antioxidant, and neuroprotective effects. **Methods:** A simple and low-cost technique was used for the first time to synthesis of zinc oxide nanoparticles (znonps) using *Martynia annua* leaf extract (MAE) as a reducing, mapping and stabilising agent. The biosynthesised nanoparticles (MAE-znonps) were characterized using UV-Vis, FT-IR, SEM, PSA, XRD, and ZP techniques. Molecular docking study were performed to evaluated binding affinities of test compounds compared to metformin. Also evaluated antidiabetic activity in STZ-induced diabetes in rats. **Results:** The UV-Vis spectra of MAE-znonps exhibited a peak around 320 nm, while SEM and XRD confirmed an irregular crystalline structure. In the DPPH assay, the IC₅₀ values for MAE-znonps and ascorbic acid was found to be 7.89 and 5.37 µg/ml respectively. In ABTS assay, IC₅₀ values of MAE-znonps and ascorbic acid was found to be 8.68 and 5.97 µg/ml respectively, indicating significant antioxidant potential. Molecular docking studies revealed that Cyclo-passifloic acid B (-8.46 kcal/mol) and Panaxatriol (-7.65 kcal/mol) exhibited higher binding affinities than metformin (-7.10 kcal/mol). In *in-vivo* studies demonstrated that MAE-znonps exhibited significant antidiabetic activity and alleviated diabetic nephropathy. **Conclusion:** The results suggests that MAE-znonps are a promising candidate for therapeutic applications in managing diabetes and related complications, offering a novel approach to a drug delivery and treatment.

Keywords: *Martynia annua*, Antioxidant, Zinc Oxide Nanoparticles, Diabetes, Streptozotocin.



PHA-BT-049: Evaluation of neuroprotective potential of sigma-1 receptor agonists in alzheimer's disorder

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Alzheimer's disease (AD) is a prevalent neurodegenerative disorder characterized by the accumulation of amyloid plaques and neurofibrillary tangles, leading to progressive cognitive decline. Current treatments primarily offer symptomatic relief, underscoring the need for new neuroprotective strategies. One promising target is the Sigma-1 Receptor (SIR), a multifunctional protein located at the mitochondrion-associated endoplasmic reticulum membrane, known to regulate cellular survival pathways and support neuronal health.

This study aims to identify potential SIR agonists from the ZINC database, focusing on FDA-approved and investigational compounds. Using Schrodinger software, a molecular docking study was conducted at the 6DKI active site, and the top-scoring compound, ZINC000095619101, was selected for further evaluation. Molecular dynamics simulations predicted a stable binding of the compound to SIR. Subsequently, in vivo assessments were carried out using AD-induced Wistar rats to determine neuroprotective efficacy.

Behavioral studies, histopathological analysis, and biochemical assays were performed to assess cognitive function and neuronal integrity. The selected compound demonstrated significant neuroprotective effects, potentially mediated through the activation of the PI3K/Akt/mTOR signaling pathway. This pathway is known to inhibit inflammatory responses and promote neuronal survival.

In conclusion, ZINC000095619101 shows promise as a therapeutic agent for Alzheimer's disease by targeting SIR and enhancing neuroprotective signaling. However, further research is necessary to pinpoint the specific genes and proteins involved in this mechanism and to validate its clinical relevance.

Keywords: Alzheimer's disease (AD), Sigma-1 receptor (S1R), Neuroprotection, Molecular Docking



PHA-BT-050: To evaluate the protective effect of novel glitazones as anti-parkinson's agents by in-vitro and in-vivo studies

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Background: Parkinson's disease (PD) is a progressive neurodegenerative disorder marked by the loss of dopaminergic neurons and α -synuclein accumulation in the substantia nigra. Parkinson disease is characterized by Lewy body formation, dopamine depletion in the striatum, and neuronal loss, leading to motor and non-motor symptoms. Research focuses on targeting peroxisome proliferator-activated receptor-gamma (PPAR- γ) and its coactivator PGC-1 α to enhance neuroprotection. Glitazones, PPAR- γ agonists, show promise in reducing inflammation, oxidative stress, and dopamine depletion, but their side effects necessitate safer derivatives.

Objectives: To evaluate the neuroprotective effect of novel glitazones, particularly compound 9j, in a 6-OHDA-induced Parkinson's disease rat model. To assess the compound's efficacy in reducing neurodegeneration and oxidative stress, improving motor functions, and confirming their safety through toxicity studies.

Methods: The study used molecular docking to identify glitazones 9j and 13d as PPAR- γ agonists. An experimental in vivo study was conducted on 6-OHDA-induced Parkinson's disease in female Wistar albino rats. Rats were divided into 7 groups and treated for 21 days following 21 days of disease induction. Behavioural tests (rotarod and locomotion) evaluated motor function. Biochemical assays measured oxidative stress markers (SOD, CAT, GSH, LPO). Histopathological studies assessed liver toxicity and neuroprotection. Conducted at JSS College of Pharmacy, Mysuru, the study aimed to assess compound 9j's efficacy in reducing neurodegeneration, oxidative stress, and confirming safety.

Results: Treatment with glitazone 9j significantly improved motor coordination and locomotor activity, especially at 30 mg/kg, showing superior efficacy over lower doses and standard treatment. Oxidative stress was reduced, evidenced by decreased lipid peroxidation and increased levels of SOD, CAT, and GSH. Histopathological analysis revealed marked neuroprotection at higher doses, with preserved neuronal structure and minimal gliosis. Liver sections showed no signs of hepatotoxicity, confirming compound safety. Compared to the disease control, 9j-treated groups showed reversal of neurodegeneration. Overall, glitazone 9j demonstrated strong neuroprotective, antioxidant, and safe therapeutic potential for managing Parkinson's disease in the 6-OHDA rat model.

Conclusion: Glitazone 9j exhibited significant neuroprotective and antioxidant effects in a 6-OHDA-induced Parkinson's disease rat model. It improved motor functions, reduced oxidative stress, and showed no hepatotoxicity. These findings suggest that 9j is a promising and safe therapeutic candidate for managing Parkinson's disease and warrants further clinical investigation.

Keywords: Glitazone 9j, Parkinson's disease, Neuroprotection, Oxidative stress, PPAR- γ agonist, 6-OHDA rat model



PHA-BT-051: Zein-Coated Roflumilast Nanoemulsion attenuates neuroinflammation in LPS-induced Alzheimer's Disease Model

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Background: Current therapeutic strategies for Alzheimer's disease (AD) remain symptomatic, necessitating the exploration of novel targets. Among the multi-factorial pathways for neuroinflammation in AD progression, phosphodiesterase-4 (PDE4) inhibition is emerging as a promising therapeutic strategy. In this study, Roflumilast, FDA-approved PDE-4 inhibitor was investigated for its potential neuroprotective effects in AD. Further, to mitigate systemic adverse effects, an intranasal nano emulsion formulation was developed.

Aim & Objectives: To evaluate the potential of Zein-coated Roflumilast Nanoemulsion for enhanced brain targeting and in attenuating neuroinflammation in LPS-induced Alzheimer's disease (AD) models.

Methodology: The study employed a multi-modal approach beginning with in-silico analysis using Schrödinger Suite (2022-1) to perform molecular docking and dynamic simulations of Roflumilast-PDE4 interactions, assessing binding affinity and complex stability. Subsequently, Zein-coated Roflumilast nanoemulsion (ZR-NE) was developed using Lauroglycol 90 as the oil phase and Tween 80/Ethanol as surfactant/co-surfactant system, with comprehensive characterization including particle size, PDI, zeta potential, and *in vitro* release. The *in vivo* studies were conducted to assess neuroprotective effects using two models: a transgenic AD model in *Drosophila melanogaster* (UAS-ELAV-GAL4 expressing Amyloid- β gene) and LPS-induced AD in Wistar albino rats.

Results: In silico analysis demonstrated roflumilast's strong binding affinity for the PDE4B2 isoform. *In vivo* validation using a *Drosophila* AD model showed significant improvement in negative geotaxis performance and elevated brain antioxidant levels. An Intranasal ZR-NE effectively reduced Alzheimer's disease-like symptoms *in vivo* model using LPS-induced Wistar Rats, as seen by increased alternation activity, decreased escape latency, and improved recognition index. These results were corroborated by biochemical estimations, which showed a reduction in oxidative stress and histopathological evaluation.

Conclusion: Our study suggests that Intranasal ZR-NE can be a promising drug delivery system for AD treatment. Further investigation related to brain occupancy and underlying mechanisms is warranted to strengthen our current findings.

Keywords: Alzheimer's disease; Intra-nasal; Neuroinflammation; Phosphodiesterase 4B; Roflumilast



PHA-BT-052: Butterfly Pea and the Kidney: Uncovering the Renoprotective and Renocurative Effects of *Clitoria ternatea* in Gentamicin-induced Renotoxicity Model.

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Background: The kidneys are particularly susceptible to toxic injury due to their high exposure to circulating substances, especially from drugs like gentamicin, which causes nephrotoxicity by accumulating in proximal tubules and inducing reactive oxygen species. No adjuvant therapy is currently established to mitigate this. *Clitoria ternatea*—an Ayurvedic herb is traditionally used to treat various ailments and may offer nephroprotective benefits.

Aims & Objectives: To evaluate the prophylactic and curative effects of ethanolic *Clitoria ternatea* extract on gentamicin-induced renal toxicity in rats.

Methods: Thirty albino Wistar rats were randomized into five groups: Group I (normal control), Group II (toxic control with gentamicin 40 mg/kg/day), Groups III and IV (prophylactic groups receiving gentamicin with 500 or 1000 mg/kg extract), and Group V (curative group receiving gentamicin followed by 1000 mg/kg extract from day 14 to 21). Biochemical parameters—including serum/urine creatinine, blood urea nitrogen, GSH, catalase activity, and lipid peroxidation—were measured. Histopathological evaluation was performed on day 22.

Results: Group IV demonstrated optimal efficacy; thus, its dose was selected for curative treatment in Group V. Treated animals showed significant reductions in serum/urine creatinine ($p < 0.05$), BUN ($p < 0.01$), and lipid peroxidation reduced up to 47%, with increased GSH up to 71% and catalase activity to 63%. Histological analysis revealed preserved renal architecture with reduced necrosis and inflammation.

Conclusion: Thus, the study confirms that the ethanolic extract of *Clitoria ternatea* exhibits potent renoprotective and renocurative properties through its antioxidant and anti-inflammatory mechanisms. GC-MS analysis revealed therapeutically active compounds, Pterocarpin and Homoptercarpin, which may contribute to its therapeutic effects.

Keywords: Gentamicin, Renoprotection, Glutathione (GSH), Catalase, and Oxidative stress.

PHA-BT-053: Safer CDK4/6 Therapies: Bridging Computational Toxicology to Clinical Outcomes

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Background: CDK4/6 inhibitors—including abemaciclib, palbociclib, and ribociclib—have significantly advanced the treatment of hormone receptor-positive breast cancer by disrupting cell cycle progression. Despite their clinical success, concerns about off-target interactions and associated toxicities remain a barrier to optimized, patient-specific therapy. Computational toxicology offers a strategic framework to anticipate and minimize these adverse effects through detailed molecular-level profiling. This study employs state-of-the-art in silico techniques to evaluate the safety landscape of CDK4/6 inhibitors, aiming to support the development of more selective and tolerable treatments aligned with the goals of precision oncology.

Aims & Objectives: This study aims to enhance the safety of CDK4/6 inhibitors for breast cancer by identifying and comparing their off-target profiles and toxicity risks using computational toxicology tools and database mining.

Methods: A comprehensive in silico framework was applied to examine the off-target interactions and potential toxicity of the CDK4/6 inhibitors Abemaciclib, Palbociclib, and Ribociclib. Potential non-CDK targets were predicted using reverse pharmacology platforms such as pharmlmapper, swisstargetprediction, and PASS, etc. These predicted targets were then cross-referenced with adverse event data from CTD and SIDER databases to link them with toxicities, including diarrhea, hepatotoxicity, fatigue, and neutropenia. STRING and Gene Ontology (GO) enrichment analyses were used to explore biological pathways associated with toxicity. Literature curation further supported key associations, facilitating a comparative assessment of the safety profiles of the three inhibitors for precision oncology applications.

Results: Computational profiling revealed distinct off-target interactions for Abemaciclib, Palbociclib, and Ribociclib. Abemaciclib exhibited broader kinase promiscuity, potentially explaining its higher GI and inflammatory toxicity. Palbociclib and Ribociclib showed greater specificity, with off-targets linked to hematological toxicities. Toxicity mapping identified associations with adverse effects such as diarrhea, hepatotoxicity, fatigue, and neutropenia. Enrichment analysis highlighted pathways related to apoptosis, oxidative stress, and immune response. Literature evidence supported key off-target–toxicity links, enabling a comparative safety assessment of these inhibitors.

Conclusion: This study highlights the value of computational toxicology in differentiating the off-target profiles and toxicity risks of CDK4/6 inhibitors. Abemaciclib showed a broader off-target landscape, potentially linked to gastrointestinal and inflammatory effects, while Palbociclib and Ribociclib were more associated with haematological toxicities. These insights support the integration of in silico profiling into early drug evaluation to guide safer, more targeted therapeutic decisions in breast cancer treatment.

Keywords: Abemaciclib, CDK4/6 inhibitors, off-targets, computational toxicology, reverse screening, breast cancer, adverse effects, pharmacovigilance, precision medicine

PHA-BT-054: Targeting the untapped KDEL pathway: to modulate UPR signaling and reduce ER stress in the rotenone-induced PD model

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Introduction: Parkinson's disease (PD) involves dopaminergic neurodegeneration and ER stress due to UPR dysfunction. This study explores Citicoline's potential as a KDEL agonist. *In silico* docking will identify lead molecules, followed by *in vivo* evaluation in *Drosophila* and rat models to assess its neuroprotective and anti-parkinsonian effects against rotenone-induced toxicity.

Aim: Targeting the KDEL pathway with Citicoline to modulate UPR signaling and reduce ER stress in a rotenone-induced Parkinson's disease (PD) model.

Methods: A structured approach was followed: (1) *in silico* analysis using Schrödinger suite 2022-4 for virtual screening, molecular docking, ADMET profiling, and molecular dynamics simulation to identify potential KDEL-targeting molecules. (2) *in vivo* assessment in *Drosophila melanogaster*, where rotenone-induced pd was treated with Citicoline, analyzing survival rates, locomotion, and oxidative stress markers. (3) *in vivo* validation in rats, investigating citicoline's neuroprotective effects through behavioral tests (apomorphine-induced rotations, grip strength, locomotion), histopathological analysis, and biochemical assays.

Results: *In silico* screening identified Citicoline as a promising KDEL agonist with a high binding affinity (docking score: -7.94 kcal/mol; MMGBSA: -43.86 kcal/mol). Molecular dynamics simulations confirmed stable binding and strong interactions with the KDEL protein (PDB: 6I6H). *In vivo* studies are expected to show improved survival, locomotion, and reduced oxidative stress and neuroinflammation in both models.

Conclusion: Citicoline was identified as a potential KDEL agonist, showing strong binding affinity and stable interactions. *In vivo* studies in *Drosophila* and rat models are anticipated to confirm its neuroprotective effects, highlighting its therapeutic potential for PD.



PHA-BT-055: Evaluation of Nanotechnology-mediated sirna for targeting selected Genes involved in Alzheimer's Disease

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Background: Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by cognitive impairment. Cyclin-dependent kinase 5 (Cdk5) has been implicated in AD pathogenesis. Small interfering RNA (sirna)-mediated gene silencing offers a novel therapeutic approach, but its clinical translation is hindered by challenges in cellular uptake and stability.

Aims & Objectives: To develop and evaluate chitosan-PLGA-based nanoparticles for the effective delivery of sirna targeting Cdk5, aiming to enhance its stability, uptake, and gene silencing efficacy for potential AD therapy

Methods: Cdk5-targeting sirna sequences were designed using IDT tools and synthesized. Chitosan-PLGA nanoparticles encapsulating sirna were prepared using the emulsion solvent evaporation method. The formulation was characterized for particle size, zeta potential, and sirna complexation via gel retardation. Stability in serum, cytotoxicity (MTT assay on SH-SY5Y cells), and gene silencing efficiency (RT-PCR) were evaluated.

Results: The optimized nanoparticles displayed a particle size below 200 nm, positive surface charge, and strong sirna binding. They demonstrated enhanced serum stability and low cytotoxicity. RT-PCR confirmed effective silencing of the Cdk5 gene, indicating successful delivery of sirna.

Conclusion: Chitosan-PLGA nanoparticles provide a promising platform for sirna delivery targeting Cdk5 in Alzheimer's disease. The formulation effectively enhances sirna stability and gene silencing efficiency. In vivo validation using a scopolamine-induced AD model in Wistar rats will include behavioral, biochemical, and histopathological assessments.

Keywords: Alzheimer's disease, Cdk5, sirna, chitosan-PLGA nanoparticles, gene silencing, nanotechnology.



PHA-BT-056: Assessment of the Metabolic Preconditioning Induced by Snehapana Therapy in the Management of Type II Diabetes

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Background: Loss of metabolic conditioning is an essential contributor in the development of metabolic disorders. Restoring metabolic conditioning requires a multifaceted approach, including Pharmacological interventions, conventional and alternative therapies, regular physical activity and strategic lifestyle modifications. Among these techniques preconditioning is highly efficient adaptive mechanism. Preconditioning enhances adaptive response by subjecting the body to brief, moderate metabolic stress, eventually enhancing metabolic flexibility and against conditions such as type 2 diabetes.

Objectives: This study explores the effect of Snehapana therapy with normal and medicated ghee on insulin resistance in a high-fructose diet-induced type 2 diabetes model in rats, using histological, biochemical, and biomolecular analysis to assess improvements in insulin sensitivity and signalling pathways.

Methodology: Snehapana therapy was administered for 14 days at varying doses to precondition the animals' metabolism, followed by a 14-day recovery period. An OGTT and lipid profile were performed on the last day of recovery. Subsequently, a high-fructose diet was given for 6 months to induce insulin resistance, after which OGTT, lipid, and insulin levels were assessed. Animals were then randomized into 7 groups and treated with metformin alone or in combination with Snehapana (200 mg/kg) for 14 days. After another 14-day recovery, OGTT, biochemical parameters, and western blot analysis (IRS-1, GLUT-4, HSP-70, P-AMPK, and AMPK) were conducted.

Result: Cholesterol levels, triglyceride levels, SGOT levels, total protein levels, urea and insulin levels are elevated in the high-fructose diet control group, consistent with the development of metabolic dysregulation. However, this increase was notably absent in the preconditioned with Snehapana groups.

Conclusion: These findings suggest that Snehapana therapy, as a preconditioning strategy, confers resistance against the deleterious effects of long-term high-fructose diet exposure. This protective effect may be attributed to the modulation of lipid metabolism and improved systemic glucose homeostasis induced by therapeutic treatment.



PHA-BT-057: *Allamanda cathartica* L. Leaves as a hepatoprotective agent: An experimental study in ccl4 treated wistar albino rats.

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Background: Liver damage caused by certain toxins like carbon tetrachloride are a major health concerns, prompting the search for effective natural hepatoprotective agents.

Aims & Objectives: This study investigates the hepatoprotective activity of the leaves of *Allamanda cathartica* L. In carbon tetrachloride (ccl₄) induced wistar albino rats.

Methods: Powdered *Allamanda cathartica* leaves were extracted by maceration and subjected to phytochemical screening and acute oral toxicity testing (OECD 425). Ethanolic extract doses (200 and 400 mg/kg b.wt) were administered to rats with ccl₄-induced hepatotoxicity. Silymarin (50 mg/kg) served as standard. Liver function was assessed using biochemical markers (SGOT, SGPT, ALP, GGTP, glucose, bilirubin, protein, lipid profile) and antioxidant enzymes, supported by histopathological examination of liver tissues.

Results: Preliminary phytochemical screening of *Allamanda cathartica* leaf extract revealed the presence of alkaloids, cardiac glycosides, saponins, flavonoids, tannins, proteins, amino acids, sterols, triterpenoids, and carbohydrates. Acute toxicity studies confirmed the extract's safety up to 2000 mg/kg. The ethanolic leaf extract exhibited dose-dependent hepatoprotective activity by normalizing elevated biochemical markers, with results comparable to standard drug Silymarin. Histopathological findings further supported the extract's liver-protective effect.

Conclusion: The study shows that *Allamanda cathartica* leaf extract has promising hepatoprotective activity, likely due to phytoconstituents such as alkaloids, glycosides, saponins, flavonoids, tannins, proteins, sterols, and triterpenoids. Further research is needed to isolate and identify the specific active compound responsible.

Keywords: Hepatoprotective activity, *Allamanda cathartica*, Carbon tetrachloride



PHA-BT-058: Revolutionizing Cardiac Therapy: Targeted Biodegradable Magneto liposomes Entangled with Ezetimibe for Strategic Treatment for Hyperlipidemia: An In Vivo Approach

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Background: Hyperlipidemia remains a major risk factor in the progression of cardiovascular diseases, driven by elevated levels of LDL-C, total cholesterol, and triglycerides. Although standard therapies like statins and ezetimibe are clinically established, their effectiveness is often limited by systemic side effects, poor bioavailability, and lack of targeted action. Ezetimibe, a potent NPC1L1 inhibitor, reduces cholesterol absorption but faces challenges related to solubility and pharmacokinetics. Recent developments in nanomedicine have introduced magnetoliposomes—lipid-based vesicles embedded with magnetic nanoparticles—which enable site-specific drug delivery under the influence of an external magnetic field. These systems can enhance local drug accumulation in atherosclerotic tissues, minimizing systemic exposure. Encapsulating ezetimibe within magnetoliposomes offers a promising strategy to overcome its therapeutic limitations. Oral administration of this formulation improves patient compliance while preserving pharmacological activity. Dual hyperlipidemic models using high-fat diet and Triton X-100 provide a reliable experimental framework for efficacy assessment. This study aims to develop and evaluate a magnetically-targeted, orally-administered ezetimibe formulation for the strategic management of hyperlipidemia-associated cardiovascular dysfunction.

Aims & Objectives: The aim of the current study is to prepare and develop the magneto liposomes entangled with ezetimibe against cardiovascular diseases using suitable models

Objectives

1. To develop magnetoliposomes entangled with ezetimibe by employing appropriate pharmaceutical methods
2. To characterize and evaluate the developed magnetoliposomes using standard methodologies
3. To assess the toxicological profile of the test formulation using standard OECD guidelines
4. To optimize the recommended induction model to establish therapy with magnetoliposomes
5. To ascertain the ameliorative effect of the formulation by employing pharmacological evaluation methodologies

Methods: This study developed and evaluated a magneto liposome-based oral formulation of ezetimibe for the treatment of hyperlipidaemia and its associated cardiovascular complications. Magneto liposomes were prepared using phosphatidylcholine, cholesterol, and Fe₃O₄ magnetic nanoparticles, along with stabilizers like PEG and surfactants. The drug was incorporated into the lipid phase, and hydration was performed using a magnetic nanoparticle solution under controlled conditions. The formulation was assessed for particle size, zeta potential, entrapment efficiency, drug release profile, and morphology using TEM and DLS.

Acute oral toxicity was evaluated in Albino Wistar rats according to OECD guideline 423. Hyperlipidaemia was induced using a high-fat diet and Triton X-100, followed by treatment with ezetimibe-loaded magneto liposomes. Pharmacological evaluations included lipid profile



analysis, cardiac biomarkers (CK-MB, LDH, Troponin I), antioxidant enzyme activity (SOD, CAT, GSH, MDA), and histopathological assessment of cardiac tissues using Oil Red O and H&E staining.

Results: The magnetoliposome formulation exhibited nanoscale particle size (150–200 nm) with uniform distribution, high drug entrapment efficiency (>80%), and sustained release of ezetimibe. In vivo studies showed significant improvement in lipid profiles, including reductions in LDL-C, total cholesterol, triglycerides, and increases in HDL-C levels. Treatment with the formulation led to reduced serum cardiac biomarkers and restored antioxidant balance, evidenced by elevated SOD, CAT, and GSH levels and reduced lipid peroxidation (MDA). Histopathological analysis confirmed reduced lipid deposition and preservation of myocardial architecture. No signs of acute toxicity or behavioral changes were observed during toxicity testing.

Conclusion: The developed oral magnetoliposome formulation of ezetimibe demonstrated promising therapeutic potential for the management of hyperlipidemia. It provided sustained drug release, effective lipid modulation, and cardioprotective effects in preclinical models with minimal systemic toxicity. These findings support the use of magnetically targeted nanocarriers as a novel and non-invasive strategy for hyperlipidemia-associated cardiovascular disease.

Keywords: Hyperlipidemia, Ezetimibe, Magnetoliposomes, Triton X-100, High-Fat Diet, Cardiac Biomarkers, Antioxidants, Oral Nanocarrier, Targeted Drug Delivery, Cardiovascular Disease

PHA-BT-059: Isolation, Characterization and Evaluation of putative probiotics for the treatment of colon cancer

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Introduction:

Probiotics are live microorganisms that confer health benefits to the host by aiding digestion, enhancing immune responses, and suppressing harmful gut pathogens. Among them, strains exhibiting enzymatic activity, antimicrobial effects, and anti-cancer potential are of particular interest for therapeutic use. This study investigates the probiotic strain CIM S2, focusing on its functional efficacy, safety, and possible role in colon cancer management.

Objective: The primary objective was to evaluate CIM S2 for its enzymatic functions, antimicrobial properties, and in vitro anti-cancer potential, with an emphasis on its application in digestive health and colon cancer prevention.

Methodology: Functional assessment involved analyzing key enzyme activities such as protease, lipase, and amylase. Antimicrobial potential was examined through bacteriocin production, biofilm formation, hydrogen peroxide generation, and cholesterol-lowering ability. Safety was evaluated by screening for biogenic amine production and dnase activity. Anti-cancer activity was assessed via MTT assay using HCT-116 colon cancer cell lines to determine effects on cell viability.

Results: CIM S2 showed significant enzymatic activity supporting digestive function. It also exhibited notable antimicrobial effects, including bacteriocin secretion, strong biofilm production, and cholesterol reduction. No biogenic amines or dnase activity were detected, confirming the strain's safety. Notably, CIM S2 significantly decreased the viability of HCT-116 cells, suggesting anti-cancer potential.

Conclusion: CIM S2 demonstrates promising multifunctional probiotic traits with potential benefits for gut health and colon cancer management. Future in vivo and molecular research is needed to validate these findings and support its use in therapeutic or dietary probiotic applications.

Keywords: Probiotic strain CIM S2, Enzymatic activity, Proteolytic activity, Lipolytic activity, Amylolytic activity, antimicrobial activity, Bacteriocin production, Biofilm formation, Hydrogen peroxide production, Cholesterol removal, Safety assessment, Biogenic amine analysis, dnase activity, Colon cancer inhibition, HCT-116 cell cytotoxicity, Cancer cell viability reduction, Therapeutic potential



PHA-BT-060: Evaluation of gastroprotective activity of *vigna unguiculata* (L.) Walp. Seed in rats

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Background: *Vigna unguiculata* (L.) Walp is traditionally used to treat neuritis, insomnia, weakness, cardiac conditions, diabetes, digestive disorders, urolithiasis, and hypercholesterolemia.

Aims & Objectives: The present study was designed to investigate the gastroprotective effect of ethanolic and aqueous seed extracts of *V. Unguiculata* at doses of 200 and 400 mg/kg in Wistar albino rats.

Methods: Phytochemical studies identified physiologically active ingredients. Ethanolic and aqueous extracts contained quercetin and kaempferol, according to TLC. FT-IR identified functional groups in test substances. Following OECD 425 recommendations, acute oral toxicity data from prior literature determined the safe dose. Omeprazole was used to test anti-ulcer activity in indomethacin-induced and pylorus ligation ulcer models. They assessed ulcer index, ulcer inhibition %, gastric juice volume, pH, total acidity, and free acidity. One-way ANOVA and Dunnett's multiple comparison test were used.

Results: Phytochemical screening found phenols, tannins, terpenoids, flavonoids, steroids, glycosides, alkaloids, carbohydrates, proteins, saponins, and triterpenes in both extracts. TLC detected quercetin and kaempferol. FT-IR revealed polyphenolic chemicals, aromatic amines, ketones, lipids, proteins, carboxylic acids, cyclic ethers, and aldehydes. High concentrations of both extracts inhibited ulcers in both models. High-dosage ethanolic seed extract lowered ulcer index, gastric juice volume, free acidity, and total acidity more than control and aqueous extract groups, suggesting gastroprotection.

Conclusion: The study concludes that the ethanolic extract of *Vigna unguiculata* (L.) Walp possesses significant gastroprotective activity. This effect may be attributed to the presence of flavonoids, phenolic compounds, terpenoids, steroids, saponins, polysaccharides, glycosides, and alkaloids.

Keywords: *Vigna unguiculata* (L.) Walp, anti-ulcer activity, flavonoids, pyloric ligation, indomethacin, omeprazole.



PHA-BT-061: Evaluation of Tulsi (*Ocimum sanctum*) for Diabetic Neuropathy and Associated Complications

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Background: Diabetic neuropathy is one of the most prevalent complications of diabetes, often leading to pain and cognitive impairment. Current treatment strategies primarily offer symptomatic relief rather than addressing the underlying mechanisms.

Aims & Objectives: This study aimed to evaluate the therapeutic potential of tulsi (*Ocimum sanctum*) in treating diabetic neuropathy, reducing blood glucose levels, alleviating pain, and mitigating associated complications such as cognitive impairment and gut dysbiosis.

Methods: Diabetic neuropathy was induced in mice using a high-fat diet and streptozotocin. Levetiracetam was used to treat neuropathic symptoms, while metformin was administered to reduce blood glucose levels. Tulsi aqueous extract was tested for its efficacy. Morphological, behavioral, and biochemical analyses, including the Morris water maze task, acetylcholinesterase activity, and nociception tests, were performed.

Results: Tulsi and levetiracetam demonstrated memory-enhancing and analgesic effects. Metformin lowered blood glucose levels but did not improve memory or pain symptoms. Tulsi exhibited potent antioxidant and hypolipidemic activity, showing superior efficacy compared to metformin and levetiracetam.

Conclusion: Tulsi is a promising treatment option for diabetic neuropathy, offering neuroprotective, analgesic, and hypoglycemic benefits. Further investigations in higher animal models and biomarker studies are necessary to validate these findings.

Keywords: Diabetic Neuropathy, Cognitive Impairment, Gut Dysbiosis, *Ocimum sanctum*, Nociception.



PHA-BT-062: Exploring the therapeutic potential of ethanolic extract of *Momordica dioica* leaves for Antiulcer and Anti-inflammatory activity – A preclinical Investigation

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Background: Gastric ulcers, commonly triggered by NSAIDs like aspirin, are closely linked to oxidative stress and mucosal inflammation. The imbalance between aggressive gastric factors and mucosal defenses promotes ulcerogenesis. Natural plant-based therapies with antioxidant and anti-inflammatory potential are being explored as safer alternatives to synthetic drugs. *Momordica dioica*, traditionally used in folk medicine, is one such candidate with promising bioactive properties which may offer gastro protection action.

Aims & Objectives: This study aimed to evaluate the antiulcer activity of the ethanolic extract of *Momordica dioica* leaves in an aspirin-induced gastric ulcer model in rats and to assess its anti-inflammatory potential.

Methods: Ulcers were induced in Wistar albino rats using aspirin, and the animals were pretreated with *Momordica dioica* ethanolic leaf extract. The ulcer index, gastric protection, and antioxidant parameters such as lipid peroxidation (LPO) and reduced glutathione (GSH) were assessed. Anti-inflammatory activity was evaluated using the carrageenan-induced paw edema model to determine peripheral anti-inflammatory effects of the extract.

Results: The ethanolic extract of *Momordica dioica* leaves significantly reduced gastric ulceration, with 70.8% inhibition in ulcer index. A 62.77% decrease in lipid peroxide levels indicated notable oxidative stress mitigation. Furthermore, an 85.78% increase in GSH levels demonstrated restoration of antioxidant defense. In the carrageenan-induced paw edema model, the extract showed a significant reduction in paw swelling, supporting its anti-inflammatory effect.

Conclusion: The study confirms that *Momordica dioica* leaf ethanolic extract exhibits strong antiulcer activity in aspirin-induced ulcers, likely through its antioxidant mechanism and peripheral anti-inflammatory action. The decrease in lipid peroxidation and elevation of GSH levels suggest oxidative stress modulation as a key pathway. These findings support the traditional use of *Momordica dioica* and its potential as a natural gastroprotective agent.

Keywords: peptic ulcer, oxidative stress, gastric juice, pepsin, paw edema



PHA-BT-063: Evaluation of in vitro anti-diabetic activity of ethanolic leaf extract of *Ruta graveolens* (L.)

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Ruta graveolens, a medicinal herb known for its therapeutic properties, was evaluated for its in vitro antidiabetic activity. The ethanolic extract of its leaves underwent phytochemical screening, revealing the presence of alkaloids, flavonoids, tannins, terpenoids, proteins, glycosides, and amino acids. The study employed various in vitro assays, including α -amylase and α -glucosidase inhibition, glucose uptake by yeast cells, glucose diffusion, and glucose adsorption methods. The extract demonstrated significant inhibition of α -amylase and α -glucosidase enzymes, with maximum inhibition observed at 800 μ g/ml, comparable to standard drugs such as acarbose and metformin. However, the glucose uptake assay by yeast cells showed moderate activity. These findings suggest that *Ruta graveolens* possesses potent antidiabetic properties, likely due to its rich phytoconstituent profile. The results support its traditional use and highlight its potential for development into effective herbal treatments for diabetes. Further in vivo studies are needed to confirm these in vitro results and determine their mechanisms of action.



PHA-BT-064: From LC/MS Fingerprinting to Functional Bioassays: Probing the Antibreast Cancer Activity of Quercetin Extracted from Graviola Fruit

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Background: Breast cancer remains a leading cause of cancer-related mortality among women, driving the pursuit of novel, effective therapies.

Aims & Objectives: This study investigates the anticancer potential of Quercetin 3-O- β -D-glucoside isolated from *Annona muricata* (graviola) fruit using a comprehensive LC/MS, *in silico*, and *in vitro* approach.

Methods: Preliminary phytochemical screening guided isolation of Quercetin 3-O- β -D-glucoside. LC/MS analysis confirmed the compound's identity in graviola fruit extract. *In silico* molecular docking was performed against phosphoinositide 3-kinase, topoisomerase II, and camp-dependent protein kinase to assess binding affinity. *In vitro* cytotoxicity assays were conducted on MCF-7 breast cancer cells to evaluate dose-dependent effects.

Results: LC/MS confirmed the presence of Quercetin 3-O- β -D-glucoside in the extract. Docking studies revealed high-affinity interactions with all three targets, suggesting potential multi-target engagement. MCF-7 cell viability decreased in a concentration- dependent manner upon treatment, indicating significant cytotoxic activity of the isolated glycoside.

Conclusion: Graviola-derived Quercetin 3-O- β -D-glucoside demonstrates promising anticancer properties through both computational and cellular assays. These integrated findings support further preclinical development of this phytochemical for breast cancer therapy.

Keywords: *Annona muricata*, Quercetin 3-O- β -D-glucoside, breast cancer.



PHA-BT-065: *Achillea millefolium* – A Network Pharmacology Perspective for Alcoholic Liver Disease, Non-Alcoholic Fatty Liver Disease, and Non-Alcoholic Steatohepatitis

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Background: Herbal medicines offer promising alternatives to synthetic drugs, particularly due to their lower side effect profiles and broad-spectrum efficacy. *Achillea millefolium* (yarrow), a traditional medicinal herb from the Asteraceae family, has been widely used across Europe and Asia to treat gynaecological, hepatobiliary, and gastrointestinal conditions, in addition to its anti-inflammatory and wound-healing properties. Network pharmacology, an integrative approach combining bioinformatics and systems biology, enables the exploration of complex molecular interactions and supports multi-target drug discovery, particularly useful for multifactorial diseases like alcoholic liver disease (ALD), non-alcoholic fatty liver disease (NAFLD), and non-alcoholic steatohepatitis (NASH).

Aims and Objectives: This study aims to evaluate the therapeutic potential of *Achillea millefolium* in ALD, NAFLD, and NASH using a network pharmacology approach. Objectives include: (1) Identifying active phytoconstituents and target genes, (2) Constructing protein-protein interaction and pathway-target networks, (3) Pinpointing key pathways and hub targets, (4) Screening lead compounds via molecular docking and MM/GBSA analysis.

Methods: Phytochemicals were retrieved from literature and databases. Target prediction was conducted using swisstargetprediction and superpred. Disease-associated genes were sourced from disgenet and genecards. Network analysis and visualization were performed using STRING and Cytoscape. Key targets were further validated through molecular docking and MM/GBSA analysis using the Schrödinger Suite.

Results: The network revealed multiple interactions between *Achillea millefolium* constituents and liver disease targets. Key hub proteins included STAT3, AKT1, EGFR, PIK3CA, TNF, MTOR, and nfkb1, linked to PI3K-AKT, JAK-STAT, and TNF pathways. Docking and MM/GBSA analysis identified lead compounds with high binding affinity, supporting their potential therapeutic roles.

Conclusion: This study highlights the multi-target potential of *Achillea millefolium* in managing ALD, NAFLD, and NASH, warranting further in vitro and in vivo validation.

Keywords: *Achillea millefolium*, Network Pharmacology, ALD, NAFLD, NASH, Multi-target Therapy, In Silico Docking

PHA-BT-066: Development of Intra Vaginal Gel Containing Naga Parpam and its Evaluation Using Letrozole and Testosterone Induced Rodents for the Management of PCOS

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Background: Polycystic Ovary Syndrome (PCOS) is a complex endocrine disorder characterized by hyperandrogenism, anovulation, and insulin resistance, affecting reproductive and metabolic health in women. Conventional therapies, such as metformin, exhibit limitations and side effects. Traditional Siddha medicine, particularly *Nagaparpam*, is explored for its therapeutic potential in PCOS. A novel in-situ vaginal gel formulation may enhance localized delivery and efficacy.

Aims & Objectives: This study aimed to evaluate the therapeutic potential of *Nagaparpam* formulated as an in-situ vaginal gel in a letrozole and testosterone-induced PCOS model. The objectives included formulation and characterization of the vaginal gel, induction of PCOS using hormonal agents, and evaluation of biochemical, hormonal, and morphological parameters post-treatment.

Methods: Female rats were divided into 11 groups and PCOS was induced using letrozole and testosterone. Treatment groups received in-situ vaginal gel of *Nagaparpam* at doses of 100, 150, and 200 mg/kg, while the standard group received oral metformin (20 mg/kg). Parameters like body weight, estrous cycle, serum hormone levels, lipid profile, and ovarian histopathology were assessed post-treatment.

Results: The moderate (150 mg/kg) and high (200 mg/kg) doses of *Nagaparpam* showed significant improvement in restoring estrous cyclicity, reducing androgen levels, normalizing lipid profile, and improving ovarian morphology compared to the PCOS control and even outperformed metformin in certain parameters. The low dose (100 mg/kg) showed mild improvement.

Conclusion: *Nagaparpam* formulated as an in-situ vaginal gel demonstrated promising therapeutic effects in the PCOS model, especially at moderate and high doses. This approach offers a potential alternative to conventional treatment, with enhanced local action and fewer systemic side effects.

Keywords: PCOS, Insulin resistance, *Nagaparpam*, Estrous cycle, Metformin.



PHA-BT-067: Screening of antidepressant activity of leaf extract of *Strobilanthes kunthiana*

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Background: *Strobilanthes kunthiana*, traditionally utilized in folk medicine to address immobility and various nervous system disorders, has demonstrated promising effects in the treatment of mood-related conditions.

Aims & Objectives: This research sought to assess the antidepressant effects of the ethanolic extract from *Strobilanthes kunthiana* leaves by employing established rodent models.

Methods: The Forced Swim Test (FST) and Tail Suspension Test (TST) were used on mice to see how well the extract worked as an antidepressant. The extract was given in two different amounts: 100 mg/kg and 200 mg/kg. A basic phytochemical study was done to find out if there were any active chemicals.

Result: The extract contained proteins, glycosides, alkaloids, flavonoids, carbohydrates, and tannins, steroids, according to a phytochemical study. The ethanolic leaf extract tested at 200 mg/kg had some depressive effects, but the 100 mg/kg amount had much weaker effects in both the Forced Swim Test and the Tail Suspension Test.

Conclusion: The findings demonstrate that the ethanolic leaf extract of *Strobilanthes kunthiana* exhibits antidepressant effects, which may be linked to its abundant phytochemicals, especially flavonoids, phenolic compounds, terpenoids, and alkaloids.

Keywords: *Strobilanthes kunthiana*, mood-enhancing effects, central nervous system activity, imipramine, forced swim test, tail suspension test, bioactive compounds, flavonoid content, ethanol-based extract.



PHA-BT-068: Sclareol, A labdane-diterpene alleviates insulin resistance via attenuation of low-grade inflammation; An In-vitro study

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Background: Insulin resistance is often considered a key underlying factor in the development of metabolic disorders and chronic inflammation. Tumor necrosis factor-alpha, a pro-inflammatory cytokine, has been implicated in the development of insulin resistance in obesity and type-2 diabetes. Sclareol is a labdane-diterpene reported to reduces the various metabolic disorders.

Aim & objective: The aim of this study was to examine the *in-vitro* pharmacological potential of sclareol with reference to inflammation-induced insulin resistance in skeletal muscle cells, adipocytes and pro-inflammatory cytokines inhibitory potential of sclareol against activated macrophages, an immune cell.

Methods: In the *in-vitro* study, insulin resistance condition was induced in skeletal muscle cells using Tumor necrosis factor-alpha, pro-inflammatory cytokine and these cells were treated with sclareol and the glucose concentrations were determined using the standard GOD-POD Method. Intracellular lipid accumulation assay in adipocytes (3T3-L1) was quantified by Oil Red O Staining (ORO). Inflammatory inhibition potential of sclareol was analysed using LPS stimulated peritoneal macrophages through ELISA technique and safety analysis was done using MTT assay.

Results: The results of this study demonstrated that the treatment of sclareol is able to increase the glucose uptake in skeletal muscle cells as well as inhibit the production of pro-inflammatory cytokine from activated macrophage cells and also alleviated adipogenesis without cytotoxic effect on normal mammalian cells.

Conclusion: These results suggest the suitability of sclareol for the management of insulin resistance associated metabolic disorders.

Keywords: Insulin resistance, inflammation, sclareol, *in-vitro*.



PHA-BT-069: Targeting the Endocannabinoid System in Autism: A Systematic Review and Meta-Analysis of Cannabinoid-Based Interventions

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Background: Autism Spectrum Disorder (ASD) is a neurodevelopmental condition characterized by deficits in social communication and the presence of restricted, repetitive behaviors. Conventional pharmacological treatments have limited efficacy in addressing the core symptoms and often present adverse side effects. Cannabinoid-based therapies, particularly those involving, have emerged as potential alternatives due to their neuroregulatory and anti-inflammatory properties.

Aims & Objectives: This review aims to evaluate the efficacy of cannabinoid-based interventions in individuals with Autism Spectrum Disorder (ASD). The objectives include assessing their impact on core symptoms as well as estimating pooled effect sizes for key outcomes through meta-analysis.

Methods: A systematic search was conducted in pubmed, Web of Science, and Cochrane Library up to 2025. Eligible studies on cannabinoid interventions in ASD were analyzed using a random-effects model, with heterogeneity assessed via I^2 and effect sizes calculated for continuous outcomes.

Results: Meta-analysis revealed a significant pooled improvement in social communication as measured by ADOS (Effect Size = 2.98, 95% CI: 1.28 to 4.68), while pooled SRS scores indicated a slight but significant reduction (Effect Size = -3.03, 95% CI: -5.22 to -0.83), though with high variability across studies. Autism severity, assessed via CARS, showed a moderate overall improvement (Pooled Effect Size = 14.14, 95% CI: 4.52 to 23.76). Adaptive functioning demonstrated a favorable pooled effect based on VABS scores (Effect Size = 18.57, 95% CI: 1.86 to 35.28). Heterogeneity was notable in several measures, suggesting variation in study designs, interventions, and populations.

Conclusion: Cannabinoid-based interventions show promise in improving core symptoms of Autism Spectrum Disorder, especially social communication, and adaptive functioning. Despite study variability, evidence supports their potential, highlighting the need for larger trials and future exploration of endocannabinoid system modulation.

Keywords: Autism Spectrum Disorder, Cannabinoids, Endocannabinoid System, Meta-analysis, Novel Approach.



PHA-BT-070: Association of Stroke and Migraine Among CADASIL Patients: A Comprehensive Meta-Analysis

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Background: CADASIL is a rare genetic disorder affecting the cerebral blood vessels, leading to symptoms such as migraine and stroke. Although the relationship between these two symptoms has been extensively studied, the specifics of their relationship in CADASIL are not yet clear and require further research. Despite the lack of effective treatment options that can decelerate disease progression, our study aimed to identify the primary risk factors associated with CADASIL by conducting a comprehensive meta-analysis of previously published studies.

Aim & Objectives: To evaluate the association between stroke and migraine in patients with CADASIL through a comprehensive meta-analysis.

Specific objectives are,

- To estimate the pooled prevalence of stroke and migraine in patients with CADASIL.
- To assess the association between migraine (with/without aura) and stroke risk.
- Compare clinical characteristics among CADASIL patients with migraine, stroke, or both.
- To explore potential temporal and causal links between migraine and stroke in CADASIL.
- To identify genetic and imaging correlates linked to migraine–stroke comorbidity.

Methods: A detailed literature search was performed using the pubmed, Embase, Scopus, Cochrane Review, Web of Science, and Google Scholar databases from 1990 to 2023. Studies that met the inclusion criteria and the diagnostic and outcome parameters were included. Both adjusted and unadjusted pooled odds ratios (OR) with 95% confidence intervals (CI) were analyzed.

Results: The primary analysis of six studies on CADASIL (n=1,365) revealed that migraine occurred more frequently than stroke in patients with CADASIL (OR 0.71, 95% CI 0.61-0.82, $p < 0.0001$). The secondary analysis of ten studies of migraine alone (n=56,890) showed an 83% increased stroke risk in migraine patients without aura compared to those with aura (OR 1.25, 95% CI 0.42-3.69, $p < 0.0001$).

Conclusion: Primary analysis revealed that patients with CADASIL had a higher migraine frequency than those with stroke. Secondary analysis of migraine sufferers indicated a greater incidence of stroke in patients without an aura. These findings provide crucial insights into the risk factors of stroke and migraine in CADASIL progression.

Keywords: CADASIL; Migraine with aura; Migraine without aura; Stroke;



PHA-BT-071: Psychedelics: Bridging Science, Society and Healing

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Background: Organ-on-chip (OOC), is an emerging biotechnological advancement, which has streamlined the tedious clinical drug testing, an easy process. They simulate the functions, responses, mechanisms, actions and complications of human organs, within a microfluidic biosystem (culture cell chip). Essentially, they emulate systemic biological functions to facilitate more precise and efficient drug testing.

The research on oocs dates back since 1979 when Stephen Terry created a miniaturized gas chromatograph, which laid the foundation for the creation of the first “Laboratory-on-a-chip.” In 1994, a DARPA initiative was launched to fund the development of portable microfluidic systems to detect chemical and biological weapons which in turn helped the rise of organ chips. After a few fruitful years of research, in 2014, Wyss startup Emulate was launched, leveraging the Wyss institute’s Organ chip technology to mimic human organs, in vitro, which resulted in faster, better and cheaper drug development and insights into human health. In current research, in vitro cell cultures are preferred over in vivo due to various limitations. Unfortunately, in vitro cell culturing fails to provide accurate microenvironment and in vivo cell culturing is expensive and involves ethical issues. Oocs aim to overcome these shortcomings and provide the best of both. The key component of OOC’s design is utilizing microfluids to ensure the stable concentration gradient, dynamic mechanical stress modelling and accurate construction of identical cellular microenvironment. Oocs have the advantage of complete observation and control of the system, which is impossible to recreate in in-vivo research. Multiple channels, membranes, and chambers are constructed in a polydimethylsiloxane (PDMS) array to simulate various organs on a chip. Various experiments can be performed utilizing OOC technology, including drug delivery research and toxicology. Current technological expansions involve multiple organ microenvironments on a single chip, allowing for studying inter-tissue interactions. A very well researched example is Kidney-on-a-chip. A kidney-on-a-chip has been designed, that mimics the structure and function of the capillary wall present in kidneys. Many such models are already created and research on OOC’s is advancing.



PHA-BT-072: Dissemination strategy: Taking the RAPID Model to the Masses.

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Background: Psychological First Aid (PFA) is a critical early intervention that supports individuals during crisis or disasters. The Johns Hopkins RAPID model- comprising Reflective listening, Assessment of needs, Prioritization, Intervention and Disposition- is an evidence-informed PFA framework. However its implementation remains largely confined to trained healthcare professionals, with limited public awareness or integration into community- level systems.

Aims & Objectives: To design a scalable, inclusive and culturally adaptive dissemination strategy to extend the reach and impact of the RAPID model beyond healthcare professionals to broader populations including educators, students, volunteers, and community workers.

Methods: A multi-modal dissemination framework was developed using thematic color-coded visual tools, real-life case study podcasts, community-level training resources, and mobile-based simulation learning. The strategy emphasizes storytelling, cultural customization, technology-driven engagement, and institutional partnerships. Key activities include: Development of info-graphics and videos mapped to each RAPID step using symbolic colors. Creation of a podcast series titled “RAPID Response: Stories of Psychological First Aid in Action”.

Design of a RAPID- Lite toolkit and training modules for lay responders.

Deployment of mobile- friendly interactive simulation modules for experiential learning.

Field-level pilot programs and testimonials for validation and feedback.

Results: The strategy promotes accessibility, contextual relevance, and emotional engagement. Visual tools and audio content enhance recall and relatability, while community training ensures grassroots participation. Pilot testing in educational and public health settings indicates increased awareness, improved functional application of RAPID steps, and positive reception from non-specialist participants.

Conclusion: Disseminating the RAPID model through culturally sensitive, narrative-driven, and technology-enabled formats can democratize access to Psychological First Aid. Embedding RAPID within school curricula, public health outreach, and volunteer response programs can significantly bolster societal resilience during crises.

Keywords: Psychological first aid, Reflective listening, Assessment of needs, Prioritization, Intervention and Disposition, social resilience.



PHA-BT-073: Emerging Epigenetic Interventions in Immuno-Oncology

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Background: Cold tumours are difficult to diagnose and treat due to low immune cell infiltration and minimal immunogenicity, thus posing challenge in the field of oncology theranostics. Altered epigenetic mechanisms have been identified as key attributes in cancer progression and immune evasion.

Aims & Objectives:

This conceptual poster explores the role of epigenetic modulators in converting cold tumours into hot tumours. The objective of the work is to provide an insight into the emerging epigenetic interventions in immuno-oncology to improve cancer immunotherapy and oncology diagnostics.

Methods:

A literature review was conducted using pubmed, Scopus, and clinicaltrials.gov, focusing on studies exploring epigenetic modulators that convert cold tumours to hot, enhance antigen presentation, improve immune recognition and boost the efficacy of cancer immunotherapy approaches.

Results:

Literature review revealed that agents such as DNA methyltransferase inhibitors (dnmtis), histone deacetylase inhibitors (hdacis) can remodel the tumour microenvironment and enhance antitumour activity of the immunotherapy. These agents sensitize the tumours to immune checkpoint blockade therapies and enhance overall antitumour immune response. Emerging epigenetic interventions like EZH2 inhibitors, BET inhibitors, non-coding RNA- based epigenetic approaches and role of oncolytic viruses can play a crucial role in tumour diagnosis and subsequent immunotherapy.

Conclusion:

The combination of epigenetic modulators with immune checkpoint inhibitors shows synergistic potential. It is currently under clinical investigation and offers a promising strategy to transform cold tumours and improve cancer immunotherapy outcomes. These epigenetic interventions can be explored for early diagnosis of the tumours and personalized cancer treatment regimens.

Keywords: Epigenetic Interventions, Cold Tumours, Immuno-oncology, DNMT inhibitors, HDAC inhibitors



PHA-BT-074: Evaluation of analgesic activity of hydro alcoholic extract of solanum torvum stem in mice

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Background: Solanum torvum has a rich history of use in traditional medicine, attributed to its promising therapeutic properties. This study was designed to evaluate the analgesic activity of the hydro-alcoholic extract of Solanum torvum stem (HAESST) using validated animal models.

Methods: The hydro-alcoholic extract was prepared using the Soxhlet extraction method, followed by phytochemical screening which confirmed the presence of flavonoids, alkaloids, tannins, and saponins. Acute oral toxicity tests were conducted in mice at doses up to 2000 mg/kg, revealing no adverse effects. Based on these findings, doses of 100, 200, and 400 mg/kg were chosen for further investigations. The analgesic effects were assessed using two distinct models: Eddy's hot plate (for central analgesia) and acetic acid-induced writhing (for peripheral analgesia). Mice were organized into groups (n=6) for each test, including control, standard (Tramadol), and extract-treated groups.

Results: In the Eddy's hot plate test, the high dose of HAESST (400 mg/kg) demonstrated a significant increase in reaction time across all time intervals. The medium dose (200 mg/kg) showed effectiveness at the 15-minute mark, while the low dose (100 mg/kg) did not exhibit significant activity. In the acetic acid-induced writhing test, both the medium and high doses of HAESST substantially reduced the number of writhes, indicating an effective analgesic response, whereas the low dose was not effective. The observed analgesic effects were found to be dose-dependent in both experimental models.

Conclusion: HAESST exhibits both central and peripheral analgesic effects in mice, with activity increasing in a dose-dependent manner. These findings support the traditional use of Solanum torvum stem for pain relief and warrant further pharmacological investigation.

Keywords: Solanum torvum, hydro-alcoholic extract, analgesic activity, Eddy's hot plate, acetic acid-induced writhing, mice.



PHA-BT-075: Antibiotic Resistance and the Post-Antibiotic Era: Challenges and Innovations in Drug Development

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Background: Antibiotic resistance (ABR) has resulted into a global health crisis, threatening the effectiveness of standard treatments and risking a return to the pre-antibiotic era. Widespread misuse of antibiotics in clinical, agricultural, and environmental settings has accelerated the emergence of resistant pathogens, including MRSA, ESBL-producing E Coli and carbapenem-resistant Enterobacteriaceae. The post-antibiotic era presents unprecedented challenges to modern medicine, particularly in treating infections, conducting surgeries, and managing immunocompromised patients.

Aims & Objectives: This review aims to:

1. Examine the key mechanisms and drivers of antibiotic resistance.
2. Evaluate recent innovations and alternative strategies in antimicrobial drug development.
3. Highlight global efforts in stewardship, surveillance, and policy reform.
4. Discuss the prospects and limitations of novel technologies targeting ABR.

Methods: A narrative literature review was conducted, focusing on peer-reviewed studies, WHO reports, and regulatory guidelines from 2010–2025. Particular emphasis was done on emerging therapies, resistance-modifying agents and diagnostic advancements supporting targeted therapy.

Results: Despite a growing understanding of resistance mechanisms such as β -lactamase production, efflux pumps, and target modifications, the clinical pipeline for new antibiotics remains sparse. However, recent breakthroughs in AI-assisted drug discovery, rapid diagnostics, and precision antimicrobials (e.g., CRISPR-CAS based targeting) show promise. Non-traditional interventions such as phage therapy, micro biome modulation, and immunotherapeutics are gaining momentum. Yet, commercial, regulatory, and implementation barriers persist.

Conclusion: Addressing ABR requires a multifaceted, global response combining scientific innovation with robust stewardship. While novel drug development and diagnostics are advancing, sustained investment, policy alignment, and public awareness are essential to prevent a full-blown post-antibiotic era.

Keywords: Antibiotic Resistance, Drug Development, Post-Antibiotic Era, Antimicrobial Stewardship, Phage Therapy, Novel Antibiotics, AMR, CRISPR



PHA-BT-076: Enhancement in efficacy of Immunotherapy with Artificial Intelligence - Oncology's Major Revolution

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Background: Artificial Intelligence (AI) driven Immunotherapy is modernizing the Oncology. Therapeutic handling although cause of cancer-related deaths, alternate for traditional treatments like chemotherapy and radiation therapy frequently results in adverse events and variability in patient's outcomes. Immunotherapy shows encouraging results as an emerging conventional medicine and increase the chance of survival.

Aims & Objectives: This is a narrative review inspects how AI enhances the efficacy of immunotherapy by optimizing treatment regimens, increased accuracy of diagnosis, predictive prognosis assessment, forecast outcomes, evaluating the responses and minimize toxicity and ADR.

Methods: The methodology deals with input of data and information of immunotherapy with aspects and condition of cancer with assistance of training cohorts and validation cohorts which includes pathophysiological condition, diagnostic techniques, genetic response and elucidate the cellular behavior which leads to outcome in AI to inspect or determine the treatment of an individual/patient can treat with immunotherapy or which immunotherapy is effective accordance with condition. Prediction in efficacy of immunotherapy by identifying and visualizing the tumor cells magnified and enhanced view of cells by biopsy techniques and staining methods respectively. Advancing imaging equipment and AI- based imaging techniques provide more specification and circumstantial information for illustrating the efficacy of immunotherapy and their response, magnified study of affected cells and their configuration can improve the precision of treatment. AI helps in acquiring more precised dosing of immunotherapy to obtain the desired efficacy. AI development focuses on advanced exploration of genetic variation of individual in current trend and in advancement method of next generation sequencing can enable the explorer to evaluate the genetic variation accompanied with specific oncologic conditions. Fluid biopsy techniques had brought high intensified and accurate methodology in diagnosis of conditions in oncology and which acts as a superior alternate of traditional biopsy particularly used to monitor the progression of cancer and response of the immunotherapy. Requirement of AI assistance in sorting out the genes, phenotypes, and its variability with response of immunotherapy. As of with future concerns we should enable more experimental transparency and examine, strengthen the AI-driven ideas with relevance of clinical aspects and reduce common error based on technology

Results: Treating tumor pioneering with AI-assistance anticipated to be better able to model biological behavior and treatment response has been developing since recent years and also in future advancements would create a revolution in oncology treatment.

Conclusion: Still AI faces challenges in technical aspects, none of these are harmful and it has created an huge innovative development in future advancement and creation of successful modules with proper information leads to desired outcomes in Oncology.

Keywords: Immunotherapy, fluid biopsy, phenotypes, regimens



PHA-BT-077: From Pathogen to Prescription: How Bacteriophages Are Reimagined as Antimicrobial Therapy

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Background:

Global surveillance report shows that close to 50% of the antibiotics are becoming ineffective because of the staggering increase in antimicrobial resistance (AMR). Mainly due to misuse and overuse. This has made even first-line treatment unreliable in most situations. Ironically, the solution might be in what previously terrified us, viruses. More specifically, bacteriophages; those viruses that infect and kill bacteria are now being investigated as accurate, self-propagating devices that can bypass bacterial defenses while leaving host microbiota intact.

Aims & Objectives:

To assess and consolidate recent advancement in the discovery, engineering, and use of bacteriophages on medical and environmental platforms, with emphasis on gene editing and nanocarrier-based formulations.

Methods:

This review synthesizes findings of three high-impact studies investigating phage biology, synthetic engineering, and delivery research. Research involves CRISPR-edited phages, liposome-encapsulated and microneedle-formulated phages, and enzymes derived from phages that are potent against biofilms.

Results:

Phages are highly specific, self-propagating at infection loci, and bear negligible side effects. CRISPR reagents have made it possible to engineer programmable phages that can overcome bacterial immunity. Nanocarrier systems have increased phage stability and targeting sites. Phage display platforms are also utilized for cancer diagnostics as well as gene delivery. Environmentally, phages are employed in wastewater treatment, biofilm control, and coral reef rehabilitation.

Conclusion:

Bacteriophages are a highly potent, tunable category of antivirals ready to augment or supplant conventional antibiotics. Their combination with gene editing and nanobiotechnology presents a paradigm shift in disease management of resistant infections and microbial ecosystem management.

Keywords:

Bacteriophage, CRISPR, Antimicrobial resistance, Nanocarriers, Biotechnology, Phage therapy, Biofilm



PHA-BT-078: A review of Cancer Nanomedicine: Advances, Applications and Future Directions.

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Background: Nanotechnology improves cancer treatment through enhanced drug delivery and targeting. In spite of advances such as Doxil®, extracellular vesicles, and inorganic nanoparticles, there are still clinical translation issues for most nanomedicines.

Aim: To update and consolidate recent advancements, applications, and clinical challenges of nanocarrier drug delivery systems in cancer therapy.

Objectives:

- Comparison of major nanocarriers applied in cancer therapy.
- Analysis of targeted drug delivery systems.
- Evaluation of clinical advancement of authorized and trial-stage nanodrugs.
- Identification of challenges and opportunities in cancer nanomedicine.

Methods:

A systematic literature search was done in three important databases—pubmed, sciencedirect, and Google Scholar—published between 2020 and 2024. The initial search retrieved a total of 1,032 records. After excluding 112 duplicate records, 920 unique articles were left to be screened. The articles were screened by title and , then 892 articles were excluded and 28 full-text articles were shortlisted for thorough evaluation based on the inclusion (English-language peer-reviewed papers on cancer nanomedicine and focus on nanocarriers, targeting methods, clinical trials, or licensed drugs) and exclusion criteria (Non-oncology or non-nanomedicine studies and non-peer-reviewed or non-English literature). After full-text analysis, 8 articles passed all the eligibility criteria and were used in the final analysis of this systematic review.

Result:

Nanocarriers enhance targeted anticancer therapy, but clinical translation is still hindered by biological and regulatory hurdles. Nanomedicine holds great promise for safer, more effective treatments.

Conclusion:

Nanomedicine holds great promise for targeted anticancer therapy, but broader application is hindered by biological and regulatory hurdles. Multidisciplinary research is critical to realizing its full potential.

Key Words:

Nanomedicine, Cancer therapy, Targeted drug delivery, Nanocarriers.



PHA-BT-079: Bridging Pharmaceutical Innovation with Therapeutic Impact using CAR T-Cell Therapy

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Background:

Cancer is characterized by uncontrolled cell growth with systemic effects. Conventional therapies such as chemotherapy and monoclonal antibodies are non-specific and carry off target toxicity. CAR T cell therapy through the genetic engineering of patient derived T cells to target selectively malignant cells provides greater precision, prolonged immune surveillance, and lasting remission. Its efficacy in relapsed B cell malignancies positions it at the vanguard of personalized cancer immunotherapy, overcoming major shortcomings of conventional modalities.

Aims & Objectives:

- To illustrate how CAR T cell therapy bridges lab science with actual patient treatment.
- To examine the challenges and potential future of applying CAR T cells to diseases other than cancer.

Methods:

- Synthesizing data from preclinical and clinical studies on CAR T cell.
- Comparative analysis of FDA approved therapies and the emerging modals.
- Evaluating methods like magnetically guided delivery and oncolytic virus assisted targeting in solid tumors.

Results:

CAR T cell therapy shows good remission rates in B cell cancer, with evidence of high potential in combination regimens for solid tumors. Advancements in modular CAR design and patient specific dosing regimens are adding to improved safety and efficacy. Challenges still exist with tumor microenvironment infiltration, cytokine release syndrome and manufacturability.

Conclusion:

CAR T cell therapy has shown good remission rates in blood related cancers with newer CAR designs showing extended progression free survival beyond 13 months. These success highlights the potential of the therapy in lasting disease control.

Keywords:

Cancer, CAR T cell, immunotherapy, cytokine release syndrome, solid tumors.



PHA-BT-080: Preclinical and In Vivo Evaluation of the SUPRA CAR System: A Systematic Review of Its Modular and Tunable Potential to Enhance CAR-T Cell Therapy

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Background: Chimeric antigen receptor (CAR)-T cell therapy has revolutionized cancer treatment but faces challenges including limited control over T-cell activation, cytokine release syndrome, and antigen escape, especially in solid tumours. The SUPRA (Split, Universal, and Programmable) CAR system offers a novel modular approach to overcome these limitations by enabling tunable and logic-gated T-cell responses.

Aim and Objectives; This systematic review evaluates preclinical and in vivo studies on the SUPRA CAR system, focusing on its modularity, tunability, safety, and efficacy in enhancing CAR-T cell therapy, while also assessing its potential for future clinical translation.

Methods: Review and analysis of recent studies employing SUPRA CAR-T cells in various tumour models, focusing on tumour clearance efficacy, dose-dependent cytokine modulation, and combinatorial antigen targeting using Boolean logic gates. **Literature search:** conducted in pubmed, Medline, Embase, and Web of Science using mesh terms like “SUPRA CAR,” “modular CAR-T,” and “logic-gated CAR-T,” combined with Boolean operators. No limits were set on publication date or format. **Inclusion criteria:** preclinical or in vivo studies on SUPRA CAR systems with standardized efficacy or safety assessment measures. **Exclusion criteria:** studies lacking definitive outcome measurements, reviews/editorials without original data, or published in languages other than English. **Data collected:** study characteristics (author, year, sample size), model type (hematologic or solid tumour), SUPRA CAR construct details, logic gate configuration, zipfv concentration, outcome measures (tumour burden, cytokine levels, antigen specificity), and main results (efficacy, safety, antigen targeting range).

Results: SUPRA CAR-T cells showed potent anti-tumour activity in both hematologic and solid tumour models. Cytokine secretion was finely tunable via zipfv adaptor concentration and leucine zipper affinity, allowing controlled T-cell activation and reduced cytokine release syndrome risk. The platform enabled multiplexed antigen targeting through AND, OR, and NOT logic gates, enhancing tumour specificity and minimizing off-tumour toxicity. Competitive inhibitory zipfvs further improved safety by mitigating excessive immune activation.

Conclusion: The SUPRA CAR system represents a highly adaptable and controllable CAR-T cell platform with demonstrated preclinical efficacy and safety advantages. Its modular design and programmable logic gating hold promise for overcoming key challenges in CAR-T therapy, particularly for solid tumours and heterogeneous antigen expression.

Keywords: SUPRA CAR, CAR-T cell therapy, modular CAR, cytokine control, logic-gated CAR, tumour targeting, preclinical studies, solid tumours, hematologic malignancies



PHA-BT-081: PRISM-ML: AI-Driven Multi-Omics Insights for Alzheimer's Therapy

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Background:

Alzheimer's disease (AD) leads to progressive brain shrinkage, causing memory loss, cognitive decline, and impaired language. The buildup of amyloid-beta plaques and tau protein tangles in this neurodegenerative disorder disrupts neuronal communication, which exacerbates cognitive decline in affected individuals. The molecular mechanisms of AD, despite its significant societal impact, remain not fully understood. Traditional bioinformatics methods often overlook nonlinear patterns and regional heterogeneity in AD. To address this, we developed PRISM-ML (precision-medicine using Interpretable Systems and Multiomics with Machine Learning), an interpretable machine learning framework that integrates bulk RNA sequencing (RNA-seq) and Genome-wide Association Study (GWAS) data to identify patient-specific biomarkers, subtissue-level pathology, and drug repurposing opportunities.

Methods:

PRISM-ML analyzed transcriptomic and genomic data from 2,105 post-mortem brain samples (1,363 AD, 742 controls) across nine brain regions. A Random Forest classifier with SHAP identified individual-level biomarkers. Clustering segmented tissues into 36 subtissues, and gene-gene interaction networks revealed 262 bottleneck genes. A knowledge graph-based screening then identified FDA-approved drugs targeting these genes for potential multi-target therapies.

Results:

We identified 36 distinct subtissues and 262 critical bottleneck genes enriched in pathways involving synaptic signaling, cytoskeletal organization, and extracellular matrix organization. Knowledge graph-based screening identified revealed six FDA-approved drugs predicted to target multiple bottleneck genes and relevant AD pathways. Notably, promethazine showed reduced AD incidence (hazard ratio ≤ 0.43 , $p < 0.001$) in a cohort of over 364,000 individuals. These findings highlight the clinical relevance of multi-target strategies and reveal novel AD-cardiovascular pathway links.

Conclusion:

PRISM-ML advances personalized AD therapy by uncovering patient-specific biomarkers and subtissue-level networks, revealing six repurposable drugs with multi-target potential. This approach shifts focus from single-gene interventions to systems-level precision medicine.

Keywords:

Drug Repurposing; GWAS; Personalized Medicine; Transcriptomics; Promethazine; Bottleneck Genes; Computational Biology



PHA-BT-082: Overcoming Blood-Brain Barrier Obstacles for Targeted Drug Delivery in Parkinson's Disease.

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A neurodegenerative disorder, Parkinson's disease (PD) affects the basal ganglia of the brain which causes uncontrollable movements. Symptoms of PD includes abnormal walking patterns, akinesia, tremors, postural changes, etc. The treatment for PD involves the drug penetration in the brain, in which the Blood Brain Barrier (BBB) holds great importance. The BBB serves as a crucial barrier between the brain external and microenvironment and maintains brain homeostasis by regulating the transfer of substances between the brain and the blood. The primary aim is to develop targeted drug delivery strategies to address the challenges posed by the BBB in the treatment of PD. There are many challenges for the drugs to cross the BBB they are- the BBB has active transport proteins that pump many drugs back into the bloodstream limiting their concentration within the brain even if they cross the barrier, likewise some common medication like levodopa face metabolic barriers and can generate side effects or lose efficacy due to inefficient penetration into the brain. To overcome the problems by the efflux transporter proteins the Proteolysis- targeting chimera (PROTAC) molecules are intravenously administered for PD so that it crosses the BBB layers. In case of levodopa, it was incorporated within second near-infrared region (NIR-II) gold nanorods (aunrs) and utilised angiopep-2 (ANG) for targeted delivery through the BBB. Protacs exhibit high and moderate permeability through passive diffusion in addition levodopa drug delivery method binds to low-density lipoprotein receptor related protein 1 of BBB which eases targeted drug delivery and enhances its penetration in BBB. In summary, advanced strategies like protacs and modifications of levodopa improve drug penetration across the blood-brain barrier for Parkinson's disease treatment. These innovations enhance therapeutic efficacy and hold promise for better management of neurodegenerative disorders.

Keywords: Parkinson's, BBB, Targeted Drug Delivery, protacs, Levodopa.



PHA-BT-083: Identifying and Targeting Inflammatory Microglia in Neurodegeneration

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Background: Microglia play a dual role in Alzheimer's disease (AD), contributing to both neurodegeneration and amyloid clearance. A subset known as disease-associated microglia (DAM) displays transcriptional changes, but their functional heterogeneity remains unclear.

Aim & Objectives:

This study aims to:

- Identify and characterize functionally distinct subsets within DAM.
- Determine their relevance in AD pathogenesis.
- Explore therapeutic strategies to modulate pro-inflammatory DAM and enhance amyloid clearance.

Methods:

Transcriptomic datasets from mouse models of neurodegeneration and neuroinflammation were analyzed using Weighted Gene Co-expression Network Analysis (WGCNA) to identify modules of co-expressed microglial genes. These modules were mapped onto single-cell RNA sequencing data to identify DAM heterogeneity. Flow cytometry was employed to validate distinct DAM subsets using surface markers such as CD44 and CXCR4. Pharmacological interventions included the $\text{I}\alpha/\beta$ agonist T0901317 to promote anti-inflammatory DAM and the Kv1.3 channel blocker shk-223 to suppress pro-inflammatory DAM. Amyloid- β phagocytosis assays and immunohistochemistry were conducted to assess functional outcomes in treated 5xfad mouse models.

Results:

Two distinct DAM subsets were identified:

- **Pro-inflammatory DAM:** characterized by Tlr2, Il1b, CD44, and Kv1.3 expression, regulated by nfkb and Stat1.
- **Anti-inflammatory DAM:** enriched for phagocytic markers (Igfl, Apoe, CXCR4), regulated by $\text{I}\alpha/\beta$.
- LXR agonist increased anti-inflammatory DAM and enhanced A β phagocytosis. Shk-223 selectively suppressed pro-inflammatory DAM, promoted amyloid clearance, and improved cognitive outcomes in AD mouse models. Pro-inflammatory DAM signatures correlated with human AD pathology and preceded cognitive decline.

Conclusion:

Our findings reveal distinct DAM subtypes in AD and highlight the therapeutic potential of modulating microglial states. Targeting pro-inflammatory DAM using Kv1.3 blockers and enhancing anti-inflammatory DAM via LXR activation offers promising neuroimmunomodulatory strategies in AD.

Keywords:

Microglia, Macrophage, Alzheimer's disease, Network analysis, Kv1.3, Amyloid, Neuroinflammation



PHA-BT-084: A Comparative Review on Phytochemical, Pharmacological and Antioxidant Potential of *Acacia ferruginea* DC.: An Integrative Perspective.

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Background:

Acacia ferruginea DC. Is an endangered medicinal plant with significant ethnopharmacological relevance. This plant, extensively utilized in Ayurveda and Siddha, has exhibited several pharmacological properties, including anti-inflammatory, wound healing, neuroprotective, anti-ulcer, anti-hemorrhoidal and hepatoprotective effects. With the growing global demand for herbal medicines, the need to profile and standardize its constituents is crucial.

Aims & Objectives:

This study aims to review and integrate available data on *Acacia ferruginea* DC., focusing on its pharmacological, phytochemical, physicochemical, elemental, and antioxidant properties. The objective is to highlight its therapeutic potential and emphasize the importance of standardization in herbal formulations.

Methods:

Data were collected through structured literature review covering pharmacological investigations, phytochemical screenings, fluorescence analysis, SEM-EDS metal content profiling, FT-IR spectral analysis, and antioxidant assays including DPPH and TAA methods. Quantitative estimations of major phytoconstituents were also considered to evaluate its medicinal value.

Results:

Acacia ferruginea DC. Exhibits a wide range of pharmacological activities including anti-inflammatory, hepatoprotective, wound healing, neuroprotective, anti-ulcer, and anti-hemorrhoidal effects. Quantitative phytochemical investigation verified the existence of alkaloids (1.58%), phenolics (0.56%), and terpenoids (0.75%). Physicochemical tests showed high extractive values with ethanol and ethyl acetate solvents. Elemental profiling revealed permissible levels of Na, K, and Mg, with absence of toxic metals. FT-IR spectra confirmed functional groups, while strong antioxidant activity was observed through DPPH and TAA assays. Fluorescence characteristics further supported the compound identity.

Conclusion:

The findings of this review highlight the therapeutic richness of *Acacia ferruginea* DC. And its potential use in herbal medicine. By combining pharmacological evidence with scientific standardization techniques, this study supports its future application in safe, effective, and quality-assured natural formulations.

Keywords:

Acacia ferruginea DC., antioxidant activity, pharmacological activity, phytochemicals, standardization, SEM-EDS, FT-IR



PHA-BT-085: Translational Development of Antisense Oligonucleotide for Alzheimer's Disease

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Background:

Alzheimer's disease is characterized by the accumulation of amyloid plaques derived from amyloid precursor protein and neurofibrillary tangles formed by tau proteins. The current challenge in treating Alzheimer's is that few therapies provide genuine disease modifying effects. Antisense oligonucleotides (asos) bind to RNA and modify gene expression at post-transcriptional level by causing mrna degradation, altering splicing, or blocking translation. Recent advances have shown that Asos can be used to treat Alzheimer by targeting Amyloid precursor protein and tau.

Aims & Objectives:

- Investigate recent advances in asos based therapies for Alzheimer's disease.
- To identify key targets for asos based therapeutic intervention.
- To evaluate the delivery methods and therapeutic efficacy of asos

Methods:

Various targets, like amyloid precursor protein (APP), BACE1, tau, and microrna associated with neuroinflammation and neuronal damage, are studied for ASO therapies in Alzheimer's disease. These are chemically modified to enhance their stability and facilitate efficient delivery across the blood- brain barrier (BBB), hence improving efficacy and safety.

Results: Preclinical studies showed that asos can reduce amyloid plaques and tau protein, rescuing cell from endolysosomal-autophagy dysfunction. Early phase clinical trial showed dose-dependent reduction in CSF tau.

Conclusion:

Asos targeting APP and tau offer a mechanism-based approach to AD therapy. Their development exemplifies the translational bridge from molecular innovation to clinical application.

Keywords:

Alzheimer's disease, Antisense Oligonucleotide, Amyloid Precursor Protein, tau, RNA therapeutics, translational therapeutics.



PHA-BT-086: Stem Cells Isolated from Human Dental Pulp and Exfoliated Deciduous Teeth as a Therapeutic Approach in Neurodegenerative disorders

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Background: In neurodegenerative disorders, nerve cells in the brain and spinal cord degenerate, and become irreplaceable. There are no cures for most neurodegenerative diseases, but treatments aim to manage symptoms and slow down the progression. Although Cell-therapy is an approach that involves transplanting stem cells from embryos and adult tissues into the body to replace or repair damaged nerve cells, the embryo stem cells raise ethical concerns and human stem cells need to be reprogrammed to differentiate into neurons.

Aims and Objectives:

Dental pulp is the soft tissue inside the teeth with DPSC (Dental-Pulp Stem Cells from adult molars) and SHED (Stem cells from Human Exfoliated Deciduous teeth) found in naturally fallen out milk teeth. These tissues can be utilized as therapy in neurodegenerative disorders.

Methods:

Using specific growth factors and chemicals, dental pulp can differentiate into glutamatergic, GABAergic, dopaminergic, and cholinergic neurons, significant in diseases like Alzheimer's, Parkinson's, and Huntington's, as the dysfunction of these neurons is directly associated with the occurrence of these diseases. Serum-free media, hypoxia, and 3D culture techniques aid in their differentiation.

Results:

DPCs have demonstrated neuroprotective benefits, including improved motor abilities, reduced neuronal damage, and enhanced neuron survival. In Huntington's, dpscs helped restore motor functions and decreased necrosis, and improved cognitive abilities and promoted the regeneration of neurons in Vascular Dementia. Sheds were shown to cross the blood-brain barrier, fostering neuronal regeneration in Huntington's-Disease.

Conclusion: DPSCs and sheds, in vitro, exhibit the capacity to differentiate into neuronal subtypes that are implicated in neurodegenerative diseases. Their ability to cross the blood-brain barrier and repair neurons highlights their translational potential. Dental-pulp can be perceived as a non-invasive, ethically viable alternative to traditional stem-cell therapies, paving the way for clinical application for therapy of neurodegenerative diseases.

Keywords:

Stem cells, DPCs, sheds, Dental pulp, neurodegenerative diseases, hypoxia, Huntington's disease, Parkinson's disease, Vascular dementia, Alzheimer's disease, blood-brain barrier.



PHA-BT-087: In silico and in vivo analysis of anti-diabetic potential of α -amyrin against CPT1A gene of alloxan induced diabetes

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Objective:

The present study aims to investigate network pharmacology and molecular docking studies on anti-diabetic potential of Cordia dichotoma (CD) leaves targeted carnitine palmitoyl transferase 1A (CPT1A) against alloxan-associated diabetic rats.

Methodology: Diabetes associated genes were obtained from disgenet, while potential targets of phytocompounds were predicted using Swiss Target Prediction and Way2Drugs. Overlapping targets were further analysed through STRING, KEGG, and GO enrichment. CPT1A (PDB ID:2LE3) was selected for molecular docking, was carried out with 20 target proteins to evaluate anti-diabetic potential, and the protein structure was validated through Ramachandran plot analysis. Simultaneously, the study was conducted in male Wistar rats in which diabetes was induced with alloxan. The animals were divided into 5 groups. The normal group was given 1% tween, inducer group received alloxan 120 mg/kg, i.p, standard was administered with glibenclamide 5 mg/kg, p.o., and the test group animals received the ethanolic extract of CD at a low and high dose orally for 14 days. The antidiabetic activity was assessed through measurements of body weight, blood glucose, lipid profile (TC, TG, HDL, LDL, VLDL), and histopathological evaluation of pancreatic tissue.

Result:

Network analysis highlighted CPT1A as a key diabetes-related target. Docking studies revealed that α -amyrin had the highest binding affinity (-6.8 kcal/mol). In vivo, CD extract significantly reduced serum profiles in a dosedependent manner, with 400 mg/kg showing effects comparable to glibenclamide. Histopathology revealed regeneration of β -cells and restoration of pancreatic islets, supporting its anti-diabetic potential.

Conclusion:

CD leaf extract shows strong antidiabetic and lipid-lowering effects by targeting CPT1A and promoting β -cell regeneration, suggesting its potential as a natural diabetes therapy.

Keywords:

CD, Carnitine palmitoyl transferase 1A, Diabetes, docking, Insilco analysis.



PHA-BT-088: Neutralizing Russell's Viper Phospholipase (PLA₂) Toxin using Mini α -Crystallin (MAC) peptide

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Snakebite envenomation is a neglected tropical disease and a common cause of morbidity and mortality in Southeast Asia. Among India's "Big Four" venomous snakes, Russell's viper accounts for 42% of the reported snakebite cases. Although antivenom administration is the standard treatment, it fails to neutralize the low molecular toxins such as phospholipase A₂ (PLA₂), a major venom component with hemolytic, anti-coagulant, and oedematogenic activities. This limitation underscores the need for next-generation antivenoms.

In this study, we designed and evaluated two peptide-based PLA₂ inhibitors, mini α -crystallin (MAC) and its variant MAC-GRD, derived from eye lens crystallin. Using *in silico* molecular docking and molecular dynamics (MD) simulations, both peptides showed strong interactions with PLA₂, with docking free energies (ΔG) of -13.1 (MAC) and -12.6 kcal/mol (MAC-GRD), respectively. MD results indicated that the MAC-PLA₂ complex is more stable than the MAC-GRD-PLA₂ complex, as reflected by lower RMSD values. The interaction residues were consistent across both docking and MD simulations, supporting the stability of these complexes. However, PLA₂ activity assays using synthetic substrate revealed that neither MAC nor MAC-GRD, alone or in combination with commercial antivenom, demonstrated significant inhibition of PLA₂ enzymatic activity *in vitro*. These findings suggest that although MAC peptides strongly interact with PLA₂ and form stable complexes *in silico*, they are not effective inhibitors in their current form under *in vitro* conditions. Thus, further optimization of peptide sequences is necessary to enhance their inhibitory potential. Additional *in vitro* and *In vivo* studies will be required for validation. This would aid in developing peptide-fortified antivenoms resulting in better neutralization of low molecular mass venom toxins.

Keywords: Russell's viper, Phospholipase A₂, Mini α -Crystallin, Antivenom



PHA-BT-089: Advanced AI tools as alternative to animal testing

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Traditional animal models for toxicology and drug testing are being replaced by in vitro and in silico models, driven by regulatory changes like the FDA Modernization Act 2.0. Emerging approaches include whole-mixture and component-based testing, organotypic human cell cultures, organ-on-a-chip platforms, and computational aerosol dosimetry. 3D in vitro models, including organoids, bioreactors, and bioprinted tissues, better mimic human physiology. Machine learning and artificial intelligence are transforming toxicity assessment by enhancing predictive accuracy and optimizing experimental conditions. These technologies could accelerate drug discovery while reducing dependence on animal experiments. The integration of biofabrication, tissue engineering, and computational tools holds great promise for replacing traditional animal models.

Keywords: Alternative Methods, animal models, drug discovery

Category 6

Pharmaceutical Chemistry and Drug Discovery



PC-DD-001: Computational insights and experimental breakthroughs in identifying Next-generation Acetylcholinesterase inhibitors

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The study aimed to identify the potential acetylcholinesterase inhibitors for effective Alzheimer's treatment from existing FDA-approved drugs through a drug repurposing technique via computational tools. Further, to evaluate the anti-Alzheimer's potency of the identified drug with the help of a suitable drug delivery system through *in vivo* pharmacological studies. The molecular docking and dynamics simulation studies indicated that letrozole has a significant binding affinity of -9.6 kcal/mol and a better interaction with ache. The physicochemical properties of letrozole-encapsulated slnps (L-slnps) were characterized and confirmed. Biochemical studies revealed that L-slnps significantly decreased brain Acetylcholine esterase activity induced by scopolamine, but L-slns significantly increased ache activity compared to the Sham control group. Histopathological evaluation of brain regions revealed significant insights into the neuroprotective potential of L-slnps in an AD rat model. Treatment with L-slnps demonstrated dose-dependent neuroprotection across all studied brain regions. At a low dose (2.5 mg/kg), neuronal and glial cells in the cortical and hippocampal regions showed improved regularity, although some disorganization persisted. At a mid-dose (5 mg/kg), the histopathological architecture further normalized, with neurons and glial cells exhibiting regular arrangement and morphology akin to normal cells. The high dose (10 mg/kg) provided the most significant protection, with neuronal and glial cells displaying near-normal arrangement and morphology in the cortical, hippocampal, and SN regions. This study highlights the importance of slnps-based drug delivery systems in improving the efficacy of existing therapeutic agents in neurodegenerative conditions.

Keywords: Acetylcholinesterase, Alzheimer's, drug repurposing, solid lipid nanoparticles, Letrozole



PC-DD-002: Design, Synthesis, and Comparative analysis of Pyrimidine Derivatives Synthesised via Green Chemistry and Conventional Method for Anti-Tuberculosis Activity

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Tuberculosis (TB) is still a serious worldwide health issue, demanding the development of new and effective anti-TB medications. Tuberculosis (TB) is a common infectious illness caused by the pathogenic bacteria *Mycobacterium tuberculosis* (Mtb). The illness is most commonly spread by inhaling minute aerosolized droplets that settle in the sufferers' lungs. Pyrimidine compounds have demonstrated promise as anti-TB medicines due to their various pharmacological characteristics. This work sought to synthesis, assess, characterize, and conduct in silico experiments on new pyrimidine derivatives for anti-TB efficacy. It involved software like Chemdraw, Open Babel, and Schrodinger for in silico experiments to simulate drugs. The chemicals were made using a Claisen-Schmidt condensation reaction are purified. Structural characterization included TLC, IR, mass spectrometry, and NMR studies. The study's findings show that pyrimidine derivatives may be successfully synthesized, characterized, evaluated and analyzed in silico as possible anti-TB medicines. Using both traditional and green chemistry techniques, a total of twelve molecules were synthesized with reasonable yields ranging from 70% to 90%. Using the H37RV strain of *Mycobacterium tuberculosis*, synthesized compounds underwent evaluation via the MAB assay. Analysis of the antitubercular activity data revealed that compound 6a demonstrated moderate efficacy with a MIC of 12.5 µg/ml, while compounds 6b, 6c, and 6e exhibited notable antitubercular activity with a MIC of 3.125 µg/ml. Among the synthesized compounds, the molecular docking analysis revealed that compound 6b attained the most favourable docking score.

Keywords: Tuberculosis, Chalcone, Pyrimidine, Anti-Tubercular activity.



PC-DD-003: Design and *In Silico* Characterization of P2X7 Receptor Modulators Targeting Alzheimer's Disease

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Background: Alzheimer's disease (AD) is a progressive neurological disorder that leads to neurodegeneration, resulting in memory loss, cognitive decline, and behavioral changes. Studies have suggested the involvement of the purinergic receptor (P2X7R), an ionotropic ATP-gated receptor, in AD brain pathology. Neuroprotective actions of piperine are proven, but the exact role in the mechanism of neuroprotection is still unclear.

Aim & Objectives: Our aim is to evaluate the catalytic behavior of P2X7R through docking studies with the designed piperine derivatives.

Methods: A 3D structural model of the purinergic receptor 7 (P2X7) homology was created using the SWISS-MODEL online web server (<https://swissmodel.expasy.org/interactive>). Using *in silico* technologies such as molecular docking, total free energy calculations, ADMET predictions, and molecular dynamics simulation, the potency of 23 developed piperine derivatives that act as antagonists against the P2X7R was determined.

Results: The Ramachandran plot was used to validate the built homology model of P2X7, revealing that 94.7% of the amino acids were in the preferred region. The XP-glide (-3.80, -4.58, -5.15, -5.68, -4.45, -3.84 Kcal/mol respectively) and ΔG Bind scores (-125.12, -133.11, -129.17, -147.76, -119.70, -124.47 Kcal/mol respectively) of the 23 designed molecules were higher than the standard (XP-glide -3.86, -118.18 Kcal/mol respectively). After additional ADMET screening, molecules 19 and 20 exhibited considerable central nervous system activity as standard donepezil. Based on the interaction profile, molecule 20 was chosen for additional molecular dynamic simulation research. The measured deviation and fluctuations are within an acceptable range, indicating the stability of the complex of 20 with build model P2X7R, according to the molecular dynamic simulations, RMSD, and RMSF.

Conclusion: The study's findings may serve as a basis for the development of P2X7R antagonists, which could possibly treat AD after passing through *in vitro* and *in vivo* evaluation.

Keywords: Alzheimer's Disease, Molecular Docking, P2X7R, Homology modeling, Piperine.



PC-DD-004: Design, Synthesis and Cytotoxic Evaluation of New Coumarin Coupled Pyrazole-1-Carbothioamide Derivatives

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Background:

Breast cancer is the most frequent malignancy in women worldwide. Coumarin and pyrazole have potent anticancer activity which could be helpful for creating novel, highly effective anticancer drugs. In this study, considering the evidence of the binding of coumarin and pyrazole to the EGFR receptor, a series of coumarin-coupled pyrazole-1-carbothioamide derivatives were designed.

Aims & Objectives:

To design, synthesize and characterize new coumarin coupled pyrazole-1-carbothioamide derivatives and to evaluate their cytotoxic activity through cell line studies.

Methods:

The *in-silico* studies were performed using Schrodinger software. Molecular docking was performed against the EGFR receptor (PDB: 1M17). ADME and physicochemical parameters of the compounds were also predicted to assess their drug likeness. The compounds were further evaluated based on Lipinski's rule of five to predict their oral bioavailability. Binding free energy analysis and pharmacophore modeling was employed in this study. Substituted 3-acetyl coumarin upon reaction with benzaldehyde forms coumarinyl chalcone which undergo cyclization with thiosemicarbazide in ethanol to form coumarin-coupled pyrazole-1-carbothioamide derivatives. The synthesized compounds were characterized by IR, ¹H NMR, and Mass spectral studies. All the synthesized compounds were evaluated for cytotoxic activity through MTT assay using MDA-MB-231 cell line and antioxidant activity through DPPH scavenging assay and nitric oxide scavenging assay.

Results:

Compound KCP10 showed the highest docking score -8.444 compared to the standard doxorubicin -8.328 kcal/mol. Among the synthesized compounds, KCP10 and KCP12 demonstrated higher cytotoxic activity with IC₅₀ value 7.17 and 10.12 respectively as compared to the standard doxorubicin IC₅₀ 21.19 and also showed significant antioxidant activity compared to standard ascorbic acid.

Conclusion:

Compound KCP10 exhibits the most significant cytotoxic and antioxidant activity compared to the other synthesized compounds. Hence it can be used as a lead molecule for further synthesis as anticancer agents.

Keywords:

Breast cancer, Coumarin, Pyrazole-1-carbothioamide, Docking, EGFR, MTT assay



PC-DD-005: Computational Insights and Experimental Breakthroughs in Identifying Cutting-Edge Checkpoint Kinase Inhibitors

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Checkpoint 1 kinase (Chk1) regulates the cell cycle and facilitates DNA repair processes, which are essential for preserving genomic integrity. In breast cancer, Chk1 is frequently overexpressed, which enables tumor cells to endure DNA damage. By blocking Chk1, a crucial regulator in the development and spread of malignancies, the current study investigates the potential of natural products in finding novel treatment approaches for breast cancer. According to molecular docking, ADMET profiling, and molecular dynamics simulations, NP621 (hesperidin) interacted with important Chk1 residues like CYS87, GLU85, LYS38, and ASN135 and demonstrated good stability over 800 ns in molecular dynamics simulations. It also had a favorable binding energy of -9.6 Kcal/mol. Because of its limited solubility, hesperidin was formed into liposomes. Particle size analysis was used to describe the liposomal formulation, and FTIR, XRD, and SEM were evaluated to verify that the formulation was bound to liposomes. With an IC₅₀ of 13.52 µg/ml, the HSP-LLP formulation demonstrated remarkable cytotoxicity against the MCF-7 cell line. Additionally, 58.9% suppression in the CAM experiment was caused by inhibitory effects on angiogenesis. Wistar female rats treated with DMBA-induced breast cancer respond better to the HSP-LLP formulation, which shows promise as an agent to inhibit tumor development and improve overall health. The formulation was a viable choice for additional clinical research because of its excellent efficacy, stability, and appropriate particle size.

Keywords: Breast cancer, Molecular docking, ADMET, molecular dynamics, Hesperidin-Liposomes formulation



PC-DD-006: In Silico evaluation of Quinazolinone derivatives as Tyrosine kinase inhibitors: Molecular docking and ADME Profiling”

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Background:

Triple-negative breast cancer (TNBC), accounting for ~15% of cases, is aggressive and lacks hormone-targeted therapies. The overexpression of Epidermal Growth Factor Receptor (EGFR) in early-stage breast cancer (Stage 0) has made it a vital target for therapeutic intervention. Quinazolinone derivatives are known for their anticancer properties and potential EGFR inhibition.

Aims & Objectives:

To evaluate the binding efficiency, stability, and drug-like behavior of quinazolinone derivatives against EGFR using computational approaches.

Methods:

Selected quinazolinone compounds were docked against EGFR using Glide. Top hits were assessed via MMGBSA for binding free energy. Molecular docking and free energy calculations were performed to evaluate complex stability. ADME properties were predicted using qikprop, and pharmacophore modeling validated key interactions.

Results:

Compound R91 showed the highest docking score (-7.93 kcal/mol), better than the standard drug neratinib (-6.30 kcal/mol). MMGBSA results indicated strong binding affinity for R91 ($\Delta G_{\text{Bind}} = -55.01$ kcal/mol), with favorable van der Waals and lipophilic interactions. ADME analysis confirmed R91 met drug-likeness criteria. MD simulations revealed the R91-EGFR complex to be more stable than the neratinib complex, supported by hydrogen bonding and reduced fluctuation metrics. Pharmacophore modeling confirmed key binding features.

Conclusion:

In conclusion, compound R91 demonstrated superior binding affinity and stability with EGFR compared to neratinib, highlighting its potential as a more effective EGFR inhibitor.

Keywords:

EGFR, Breast cancer, Quinazoline, Molecular docking, MMGSBA, ADME, Neratinib



PC-DD-007: Novel Styryl-Thiazole Derivatives: Design, Synthesis, and Assessment of Anti-Inflammatory Activity

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Background: Inflammation drives serious diseases despite its crucial protective origin. Standard anti-inflammatory drugs (nsaids/COX-2 inhibitors) cause significant gastric, renal, or cardiac risks by broadly blocking protective pathways. Finding safer alternatives that effectively fight inflammation without these dangerous side effects remains a major challenge. Drugs inspired by natural origins offer immense promise here as naturally occurring compounds possess optimized bioactivity, greater biocompatibility (reducing side effects), and complex multi-target mechanisms. Their vast chemical diversity provides privileged scaffolds for novel drug design. This need drives exploration of novel chemical scaffolds with natural products serving as key molecular blueprints to overcome these limitations.

Aims & Objectives: The main objectives of this study are:

- To design novel styryl thiazole derivatives
- To characterize the synthesized compounds using spectroscopic techniques
- To evaluate the anti-inflammatory potency of the synthesized compounds using the carrageenan-induced paw edema model.

Methods: Novel styryl-thiazole derivatives were synthesized via cross-aldol condensation of aldehydes with ketone, followed by cyclization with thiourea to form the thiazole amine intermediate. This intermediate was coupled with substituted cinnamic acids to yield the final compounds. Purity was assessed by TLC and melting point, while structures were confirmed by IR and ¹H-NMR spectroscopy. All compounds were evaluated for acute anti-inflammatory activity using the carrageenan-induced rat paw edema model.

Results: All synthesized styryl-thiazole derivatives were structurally confirmed by IR and ¹H-NMR spectroscopy. Anti-inflammatory evaluation using the carrageenan-induced paw edema model revealed compounds 4b and 4e exhibited potent activity, showing significant reduction in inflammation.

Conclusion: This study demonstrates that the styryl-thiazole scaffold represents a promising class of anti-inflammatory agents. The hybridization of the styryl ketone with the thiazole amine moiety significantly influences anti-inflammatory potency and is enhanced by electron-donating substituents, with 4b and 4e exhibiting the highest activity.

Keywords: Anti-inflammatory, Styryl ketone, Spectroscopy, Thiazole amine



PC-DD-008: Probing the activity of β -Amino acids: an *In-silico* approach

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Background: β -Amino acids are a class of non-proteinogenic amino acids known for their enhanced metabolic stability, conformational rigidity, and resistance to enzymatic degradation, making them promising candidates in drug discovery.

Aims & Objectives: This study employs an *in-silico* approach to evaluate the therapeutic potential of β -amino acid-based ligands against targets implicated in breast cancer, lung cancer, and antimicrobial resistance.

Methods: Nine ligands were subjected to molecular docking using autodock Vina against nine protein targets, followed by molecular dynamics (MD) simulations and ADMET profiling. Docking results revealed notable binding affinities, with several ligands demonstrating strong interactions with key residues of their respective targets. Among them, LIG1 and LIG4 exhibited the most promising binding profiles. ADMET analysis predicted favorable pharmacokinetic and safety characteristics, with all ligands complying with Lipinski's rule of five and showing acceptable toxicity profiles.

Results: MD simulations confirmed the stability of the top protein-ligand complexes, particularly the 7Z1V-LIG1 complex, which remained stable throughout a 10 ns simulation.

Conclusion: These findings support the potential of β -amino acid derivatives as viable lead compounds for further experimental validation in oncology and antimicrobial drug development.

Keywords: β -Amino acids, Molecular docking, Molecular dynamics, ADMET, Breast cancer, Lung cancer, antimicrobial resistance.



PC-DD-009: Exploring the Neuroprotective Effects of *Sechium edule* in Parkinson's Disease: Insights from Network Pharmacology and Molecular Docking

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Background:

Sechium edule (Jacq.) Sw. Is a nutritionally and pharmacologically valuable plant widely grown in tropical and subtropical regions for its edible parts. Rich in bioactive compounds like flavonoids and polyphenols, it exhibits antioxidant, anti-inflammatory, cardioprotective, hepatoprotective, anti-diabetic, anticancer, and neuroprotective effects. It shows promise in managing metabolic disorders, infections, and cancer. Despite its broad therapeutic potential, *S. Edule* is underutilized, and future research should focus on isolating active compounds, elucidating mechanisms, and exploring clinical applications to integrate traditional uses with modern medicine.

Aims & Objectives:

To explore the potential of *S. Edule* against Parkinson's disease

Methods:

This study employed a comprehensive systems biology approach to elucidate the molecular mechanisms underlying its potential anti-Parkinson's activity. LC-MS analysis of *S.edule* fruit extract identified twenty bioactive compounds, including key flavonoids such as quercetin and rutin, as well as phenolic acids like chlorogenic acid, all known for their roles in modulating oxidative stress and inflammation—central processes in Parkinson's disease (PD) pathogenesis. Network pharmacology predicted human protein targets for these compounds using IMPAAT and STITCH databases, while PD-related genes were sourced from Genecards and NCBI, resulting in the identification of 21 overlapping genes.

Visualization through protein-protein interaction networks using STRING and Cytoscape highlighted hub proteins, including AKT1, TP53, and SNCA (alpha-synuclein), which are pivotal in neuronal survival, apoptosis, and protein aggregation. Gene Ontology and KEGG pathway enrichment analyses revealed that these identified ligand targets are primarily involved in synaptic transmission, regulation of neuronal apoptosis, dopaminergic synapse signaling, and oxidative stress response—pathways directly implicated in the neurodegenerative processes of PD.

Molecular docking studies demonstrated that quercetin, chlorogenic acid, and rutin have strong binding affinities with central PD-related proteins, suggesting their potential to inhibit alpha-synuclein aggregation, enhance neuronal survival, and reduce oxidative damage. Additionally, experimental evidence supports the antioxidant capacity of *S. Edule*, reinforcing its potential as a functional food supplement for mitigating neurodegeneration and managing Parkinson's disease.

Results:

Active compounds from *Sechium edule* fruit were identified and linked to 294 human gene targets. Comparing these 10780 Parkinson's disease-related genes revealed 21 common targets. Network and enrichment analyses highlighted key pathways involved in Parkinson's disease. Molecular docking showed strong binding of *S. Edule* compounds to Parkinson's -related proteins AKT1 and TP53, supporting their potential anti-Parkinson's activity.

Conclusion:



This study highlights the use of *Sechium edule* fruit extract and explores its therapeutic potential in Parkinson's through network pharmacology and molecular docking. Key identified target for Parkinson's include AKT1, TP53. The research fills a critical gap by pinpointing molecular targets linked to *S. Edule's* anti Parkinson's activity and emphasizes the advantage of combining computational methods to reveal both direct and indirect mechanisms. Future studies involving molecular dynamics simulations and in vivo experiments are needed to validate these findings and facilitate clinical application. This integrative approach advances understanding and supports the development of *S. Edule* as a potential nutritional therapy for Parkinson's management.

Keywords:

Sechium edule, bioactive compounds, Parkinson's, Network Pharmacology, Molecular docking, gene ontology, KEGG Pathway



PC-DD-010: Discovery of Pyrazole-Based PI3K α Inhibitors with Potent Anticancer Activity: A Computational and Experimental Study

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Background:

The phosphoinositide 3-kinase alpha (PI3K α) enzyme plays a critical role in cell survival and proliferation pathways and is a validated target in cancer therapy. Pyrazole derivatives are known for their diverse biological activities, including anticancer properties.

Aims

&

Objectives:

To design, synthesize, and evaluate a novel series of pyrazole derivatives for their anticancer activity by targeting PI3K α (PDB ID: 5DXT) using molecular docking, binding energy calculations, and biological screening, to identify promising candidates for further development.

Methods:

A series of novel pyrazole derivatives was synthesized via chalcone formation followed by cyclization using hydrazine hydrate. Structural characterization was performed using UV, MS, IR, and NMR spectroscopy. Molecular docking, MMGBSA binding energy calculations, and Induced Fit Docking (IFD) were employed to assess binding affinities. Molecular dynamics (MD) simulations for 100 ns were conducted for the most active compound. Cytotoxicity was evaluated against MCF-7 breast cancer cells.

Results:

Docking scores ranged from -6.618 to -3.116, while MMGBSA binding energies varied from -46.04 to 32.89 kcal/mol. IFD results showed enhanced binding affinities, with compound MCP scoring -7.097 and MNP -7.433. MD simulations confirmed stable binding of MNP to PI3K α over 100 ns. Biological assays revealed that MNP exhibited the highest cytotoxicity against MCF-7 cells, followed by NP. Substituents such as nitro and methyl contributed to improved binding and cytotoxic profiles.

Conclusion:

The study identified MNP as a potent PI3K α inhibitor with significant anticancer activity, supported by docking, binding energy, dynamics, and biological data. These findings suggest that MNP and similar derivatives hold potential for further in vivo evaluation as selective anticancer agents targeting PI3K α .

Keywords: Pyrazole, anticancer, docking, MMGBSA, Molecular Dynamics



PC-DD-011: Synthesis and biological Evaluation of Novel Thiophene linked-1,3,4-Oxadiazole Derivatives

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Background:

Antimicrobial resistance (AMR) poses a serious global health threat due to the misuse of antibiotics and the slow development of new drugs. To address this, novel compounds combining thiophene and 1,3,4-oxadiazole moieties were designed to target the bacterial enzyme dihydrofolate reductase (DHFR), essential for DNA synthesis. These hybrids were evaluated through computational and experimental methods for their potential antimicrobial agents against resistant bacterial and fungal strains.

Aims & Objectives:

To synthesize and characterize thiophene incorporated 1,3,4-oxadiazole derivatives and to assess their antimicrobial activity.

Methods:

A series of eight thiophene-linked 1,3,4-oxadiazole derivatives (T1–T8) were synthesized and structurally confirmed; these compounds were then evaluated by molecular docking and molecular dynamics simulations with DHFR, MM-GBSA binding energy calculations, in silico prediction of ADME properties and toxicity, in vitro antimicrobial activity assays (MIC) against gram-positive and gram-negative bacteria and fungi, and in vitro cytotoxicity testing (MTT assay) on NIH3T3 cells.

Results:

All compounds met drug-likeness criteria and demonstrated good oral bioavailability and solubility; among them, T2 and T5 exhibited the best DHFR binding when compared with the standard Trimethoprim. While T2, T5, and T6 displayed excellent antibacterial activity comparable to standard drugs, and T8, T4, T1, and T2 were highly active against fungi.

Conclusion:

The study successfully synthesized a new series of thiophene-linked 1,3,4-oxadiazole derivatives with promising antimicrobial activity. In silico analysis, binding studies, and in vitro assays confirmed their favorable physicochemical properties, binding affinities, and safety profiles. Most compounds outperformed or matched current standards (Trimethoprim, Ketoconazole) in at least one microbial assay, and all showed low cytotoxicity. These findings support further development and optimization of these scaffolds for novel antimicrobial drugs.

Keywords:

Thiophene, Oxadiazole, In-silico, antimicrobial, molecular docking



PC-DD-012: Structure-Based Docking and Identification of Triazine Derivatives as potential PARP inhibitors

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Background:

Poly (ADP-ribose) polymerase (PARP) plays a crucial role in DNA damage repair and is a key target in anticancer drug discovery, particularly in tumours with defective homologous recombination repair mechanisms. Triazine-based scaffolds have shown promising pharmacological potential, prompting their exploration as PARP inhibitors.

Aim:

To identify triazine-based compounds with potential inhibitory activity against the PARP-2 enzyme using computational methods.

Methods:

The crystal structure of PARP-2 (PDB ID: 4ZZX, resolution 1.65 Å) was retrieved and processed using the Protein Preparation Wizard in Maestro 11.8. A focused library of triazine derivatives was prepared using ligprep. Molecular docking was performed using Glide SP and XP modes. The top-ranking compounds were subjected to binding free energy calculations using the MM-GBSA method in the Prime module. Key interactions with the binding pocket residues were analyzed to assess binding efficiency.

Results:

Six triazine-based compounds were identified through molecular docking as potential PARP-2 inhibitors, showing favourable binding interactions with the active site of the target protein. These compounds demonstrated stable interactions within the catalytic domain of PARP-2.

The docking results indicated that these compounds had comparable binding affinities to the reference drug, Olaparib. Binding free energy estimations using the MM-GBSA approach further supported their potential, reflecting favourable energetic profiles for stable complex formation with the protein.

Conclusion:

The in-silico results suggest that selected triazine derivatives exhibit comparable binding characteristics to Olaparib. These findings highlight the potential of triazine scaffolds as promising leads for further development of PARP-2 inhibitors in cancer therapy.



PC-DD-013: *In-Silico* Study of Some Novel Furan Derivatives as Potential Anti-bacterial Activity Against *Staphylococcus aureus* and *Enterococcus faecalis*

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Background:

Development and design of novel drug molecules for the treatment of infectious diseases is need of the hour to overcome the problems of anti- microbial resistance. Bacterial infections represent a serious health care problem mainly due to the misuse and overuse of antibiotics.

Aim and Objective:

This study attempts to select some novel furan derivatives for anti-bacterial activity against *Staphylococcus aureus* and *Enterococcus faecalis* and deals with the synthesis of furan-azetidinone hybrid compounds as potential antibacterial agents.

Methods:

Furan is a heterocyclic compound consisting of five-membered aromatic ring with four carbon atom and one oxygen atom. Both furan and azetidinone nucleus, as known as β -lactam ring have proven to have anti- bacterial activity. Hence, fusing both the nuclei by synthesizing furan-azetidinone hybrid compounds may led to the discovery of more potent anti-bacterial agents due to synergistic effect. The protein data file was selected for Human Lanosterol 14 – demethylase, Topoisomerase-II, DNA gyrase, Penicillin binding protein, β -lactamase, Dihydrofolate reductase as target. The *in-silico* molecular docking and ADMET studies were carried out for the synthesized compound in order to predict the possible mechanism of action against the targets. The formation of the novel furan-azetidinone compounds were preliminary confirmed by the TLC, Melting point, UV spectra. All the synthesized compounds were evaluated for in vitro anti-bacterial activity by agar diffusion method.

Results:

In docking study all the compound shows good binding affinity against dihydrofolate reductase target. All the derivatives have exhibited moderate activity towards the gram-positive bacteria. The compound K3 exhibits more activity towards *Staphylococcus aureus* and compound K2, K7 and K10 exhibit more activity towards *Enterococcus faecalis*.

Conclusion:

From the present study, it can conclude that among the synthesized compounds K5 and K7 showed the maximum anti-bacterial activity.

Keywords: Furan-azetidinone, UV, IR, Agar diffusion, antibacterial



PC-DD-014: Targeting Aurora A Kinase: *In Silico* Discovery of Potent Inhibitors through Integrated Pharmacophore and Simulation Approaches

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Background:

Cancer remains the second leading cause of death globally, largely due to the uncontrolled proliferation of cells driven by dysregulated mitotic processes. Aurora A kinase (AURKA), a key regulator of centrosome maturation, bipolar spindle formation, and cytokinesis, has emerged as a crucial target for anticancer drug development.

Aims & Objectives:

This study aimed to identify novel small-molecule inhibitors of AURKA using a systematic *in silico* approach, integrating pharmacophore modelling, virtual screening, molecular docking, and simulations studies.

Methods:

A ligand-based pharmacophore model was developed using MOE software based on six potent AURKA inhibitors. The validated model was used to screen the ZINC database, yielding 774 potential hits. Top candidates were subjected to molecular docking using the AURKA crystal structure. ADMET properties, DFT-based quantum calculations, 500 ns molecular dynamics (MD) simulations and MMGBSA were performed for lead evaluation.

Results:

The pharmacophore model (Aro/hyda, Acc, Don/Acc) achieved sensitivity of 69.8%, specificity of 63.6%, and accuracy of 60.4%. Two top-scoring hits, A1 (ZINC63106872) and A2 (ZINC39272872), demonstrated better docking scores (−9.24 and −8.97 kcal/mol) than the standard MK-5108 (−7.49 kcal/mol). DFT analysis showed higher dipole moments (A1: 6.15 D, A2: 6.39 D) and smaller HOMO–LUMO gaps (A1: 0.33 eV, A2: 0.38 eV), indicating higher reactivity. The MEP plot revealed distinct donor–acceptor zones, with A1 displaying a balanced electrostatic surface and A2 exhibiting stronger electron density. MD simulations confirmed complex stability with protein RMSD around 2.8 Å and ligand RMSD of 4.0 Å (A1) and 6.0 Å (A2). RMSF values for key residues remained below 2.4 Å. MM-GBSA analysis revealed favourable binding energies: A1 (−75.34 kcal/mol), A2 (−75.13 kcal/mol), MK-5108 (−74.94 kcal/mol).

Conclusion:

The study identified A1 and A2 as promising AURKA inhibitors with superior docking scores, electronic characteristics, and dynamic stability compared to the reference compound MK-5108. These candidates have potential for further development as anticancer therapeutics targeting AURKA.

Keywords:

Aurora Kinase A, Cancer, Pharmacophore modelling, Docking, Dynamics, DFT, MMGBSA



PC-DD-015: Exploration of Dimethyl-Pyrrole Derivatives as Promising Candidates Against Tuberculosis

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Background:

Tuberculosis (TB), a persistent global health challenge, is complicated by drug resistance and adverse effects from prolonged treatment. Current anti-tubercular drugs, though effective, often lead to hepatotoxicity and other systemic complications, necessitating the search for safer, more effective alternatives.

Aims & Objectives:

This study investigates a series of synthetically accessible small molecules featuring a dimethyl-pyrrole framework. The main objectives are:

- To synthesize novel derivatives with structural modifications,
- To characterize them using standard analytical techniques,
- To conduct preliminary screening for anti-tubercular activity.

Methods:

Novel dimethyl-pyrrole derivatives were synthesized via reflux of substituted aldehydes with dimethyl-pyrrole benzo-hydrazide in glacial acetic acid, followed by ethanol processing. Purity was confirmed by TLC and melting point analysis. Structures were characterized using IR, ¹H-NMR, and elemental analysis. Anti-tubercular activity was evaluated through the MABA assay against *M. Tuberculosis*. To complement biological screening, in silico molecular docking was conducted against key TB targets to predict binding affinities and interaction mechanisms.

Results:

Among the synthesized compounds (PRS:1–4), PRS-1 exhibited the most significant anti-tubercular activity. Structural modifications appeared to influence the biological activity, with specific substitutions enhancing efficacy. Docking scores aligned with in vitro activity, suggesting potential target-specific inhibition.

Conclusion:

The study underscores the potential of dimethyl-pyrrole-based molecules as a scaffold for future anti-tubercular drug development. Early findings are promising and warrant further investigation, including advanced pharmacological studies, toxicity evaluation, and mechanistic insights. These results contribute to ongoing efforts in the design of novel therapeutics for TB management.

Keywords: Tuberculosis, dimethyl-pyrrole, anti-tubercular agents, drug discovery, molecular scaffolds, resistance.



PC-DD-016: Docking-Based Identification of Quinoline Derivatives as PDGFR Inhibitors Chaitali S Prabhu Tendulkar^{a, b}, S G Vasantharaju^a

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Background:

Platelet-derived growth factor receptors (pdgfrs) play a major role in the growth and spread of tumors, especially through their role in forming new blood vessels (angiogenesis). Because of this, they've become important targets in cancer treatment. However, current drugs that block these receptors, known as tyrosine kinase inhibitors (tkis) often face challenges like resistance and unwanted side effects. This highlights the need for new, more selective therapies.

Aims & Objectives:

The objective of this study is to evaluate quinoline derivatives as potential PDGFR inhibitors using molecular docking. By predicting their binding affinity and interactions, we aim to identify promising lead compounds for further development as targeted anticancer agents.

Methods:

The crystal structure of PDGFR was prepared and refined using Schrödinger Maestro software. A focused library of quinoline derivatives was constructed and subjected to Glide XP docking. Docking scores and binding free energies were compared with the reference drug Imatinib. Protein-ligand interactions at the active site were analyzed to assess the key interactions. ADME properties of the compounds was studied by using the qikprop module.

Results:

The designed compounds showed stronger binding affinity comparable with that of Imatinib. Predicted binding poses showed strong interactions with critical residues in the PDGFR active site. The key amino acid interactions seen were comparable to those seen with the standard drug Imatinib, highlighting their potential for promising inhibitory activity against PDGFR.

Conclusion:

The *in-silico* results support the potential of quinoline scaffold as novel PDGFR-targeting agents with anticancer activity. The identified top-ranking compounds warrant further synthesis and biological evaluation to validate their anticancer potential.

Keywords: Docking, PDGFR, quinoline, anticancer



PC-DD-017: Fragment-Based Design of Novel Non-Covalent WRN Helicase Inhibitors for Targeted Cancer Therapeutics

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Background: Werner syndrome helicase (WRN), A recq family helicase involved in DNA replication, repair, and recombination, has been linked to genomic instability and an increased risk of cancer due to its dysfunction. Currently, there are no FDA-approved WRN inhibitors; there is an unmet therapeutic need, although its dysfunction increases the risk of cancer and genomic instability.

Aims & Objectives: To use computational tools and fragment-based drug discovery to identify and optimise new non-covalent WRN inhibitors.

Methodology: A fragment-linking technique was used in the current study to create novel WRN inhibitors using Schrödinger software. A total of 3,38,580 fragments of chemical libraries were examined and reduced to 2,69,302 compounds by applying the rule of three using rdkit. Following SP docking, these compounds were reduced to 13,623 based on SP docking score (≤ -7 k/cal/mol). The fragment joining produced 100 compounds, which underwent ligand preparation to produce 500 compounds. The XP docking was performed; the top 7 compounds were identified based on a docking score (≤ -12 k/cal/mol) and ligand efficiency (≤ -0.3). The best seven molecules were investigated for their ligand-receptor complex stability through a Molecular Dynamics (MD) study using Desmond software and qikprop to assess their ADME properties.

Results: Through MD and binding free energy analyses, the top seven WRN inhibitors demonstrated strong affinities and stable binding, and promising drug-like characteristics as non-covalent WRN inhibitors.

Conclusion: The Fragment-based approach identified seven promising non-covalent WRN helicase inhibitors. A thorough computational process, which included fragment screening, molecular docking, ligand efficiency evaluation, and MD simulations, was incorporated to choose WRN inhibitors. MD simulations of these compounds showed stable interactions with WRN. Their inhibitory activity and therapeutic potential against WRN-related genomic instability and cancer, however, require additional experimental validation, including in vitro and in vivo testing.

Keywords: ADME, fragment-based drug design, molecular docking, molecular dynamics, non-covalent inhibitors, WRN



PC-DD-018: Oleanolic acid Derivatives in Anticancer Therapy: Synthesis, Characterization, and Anticancer Evaluation

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Background: Oleanolic acid (OA) is a naturally occurring tetracyclic triterpenoid which can be extracted from more than 1600 different plant varieties. It has various therapeutic benefits including anticancer, anti-inflammatory, antimicrobial, wound healing, anti-diabetic, antioxidant. OA is known to induce apoptosis in cancer cell through various pathways. Even though OA is known for its anticancer property, but its effect is limited due to poor solubility, bioavailability and poor drug targeting, so to improve its pharmacological profile, we formulated OA derivatives to improve cellular uptake and increase potency against cancer cells.

Aims & Objectives:

To synthesis and evaluate oleanolic acid derivative for enhanced anticancer activity

- To synthesize and characterize oleanolic acid derivatives
- To evaluate its anticancer potential through *in vitro* assay

Methods:

OA derivatives were synthesized via structural modification to improve the anticancer potency. The compounds after synthesis were characterized using mass spectrometry, NMR and FT-IR. *In vitro* cytotoxicity assay was evaluated using MTT against cancer cell lines- MCF 7, A549, SSC9 and C6. IC₅₀ values were evaluated against the parent compound OA and among them one cell line was selected for further comparative assays with OA, like cell cycle, colony formation assay, scratch assay.

Results:

The synthesized derivatives were successfully characterized. Mass spectrometry data confirmed expected molecular weight, both ¹H NMR and ¹³C NMR showed well resolved proton and carbon signals consistent with the proposed structure and FT-IR revealed characteristic peaks corresponding to the relevant functional groups, confirming successful synthesis of the compounds. In MTT assay on MCF7, A549, SSC9 and C6, MCF7 showed better results compared to the other cell lines having IC₅₀ of OA around >100 μ M and OA1 and OA2 exhibited IC₅₀ around 10 μ M, which shows the efficacy of our synthesized compounds. Further Colony formation assay demonstrated significant reduction in colony within 14 days after OA1 and OA2 treatment more than OA itself. And cell cycle assay revealed arrest in OA1 and OA2 treated cells supporting its antiproliferative property. In scratch assay, treated cells inhibited cell migration, indicating anti-metastatic potential.

Conclusion:

OA derivatives were synthesized successfully and after preliminary anticancer evaluation, it has shown potent anticancer effect better than OA itself.

Keywords: Anticancer, bioavailability, cell viability, oleanolic acid, synthesis



PC-DD-019: In-silico Design of some novel 9-Anilinoacridine derivatives as HER2 inhibitors for anti-Breast Cancer activity

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Background: Breast cancer is the most prevalent cancer and second leading cause of cancer deaths in women (below 40 years), with an estimated 2.3 million new cases diagnosed yearly. The Human Epidermal Growth Receptor2 (HER2) When HER2 is overexpressed assumes a vital role in the pathogenesis of various human cancers making it a key target for drug development. 9-anilinoacridines play an important role as antitumor DNA-intercalating agents, due to their antiproliferative properties

Aims & Objectives: This study aims to identify potent inhibitors of the HER2 using in-silico methods to streamline drug discovery.

Methods: In the present study, for identification of potential ligands of 9-anilino acridines as selective HER2 inhibitors (3PP0.pdb) targeting breast cancer by using Schrodinger suit-2024-2, Maestro 14 version. Docking was performed by Glide module, in-silco ADMET screening by qikprop module, free binding energy was calculated by Prime-MMGBSA module and MD simulation by Desmond Module

Results: The 9-anilinoacridine derivatives AT1- AT10 have good binding affinity with Glide score in the range of -3.79 to -8.94 Kcal/mol when compared with the standard tamoxifen (-3.78). The ADMET screening of the designed molecules are within the recommended values. MM-GBSA binding results of most potent inhibitor displayed stable and favorable. A 100ns MD simulation study also confirms the stability of docking complex. Docking revealed strong ligand binding affinities at various residues. Molecular dynamics confirmed the stability of promising protein-ligand complexes

Conclusion: The results reveal that, this study provides evidence for consideration of valuable ligands in 9-anilinoacridine derivatives as potential HER2 inhibitor and contributing to advancements in targeted cancer therapies through computational methods.

Keywords: HER2 Inhibitors, Breast cancer, 9-Anilinoacridines, In-silico design



PC-DD-021: Pharmacological screening of Trk receptor agonists in Parkinson's disease

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Background – PD is a complex, progressive neurodegenerative disorder, currently recognized as fastest-growing disease globally, with an estimated 13-million individuals projected to be affected by 2040. Pathological hallmarks include progressive loss of dopaminergic neurons and neurotransmission in snpc, accompanied by accumulation of α -Syn aggregates and formation of Lewy bodies. However, beyond dopaminergic depletion, multiple converging molecular mechanisms such as mitochondrial dysfunction, oxidative stress, neuroinflammation are simultaneously involved in pathological progression. Notably, a significant reduction in the expression and signaling of neurotrophins; key regulators of neuronal survival, maintenance, and functional integrity of further exacerbates vulnerability and impairs the brain's intrinsic capacity for neuro-repair. Conventional therapies available are predominantly dopamine based, treating symptomatic manifestations, while underlying disease pathology widely being overlooked. This narrowed approach underscores an urgent need for strategies that particularly restores neurotrophin activity and signaling to enhance neuronal resilience, plasticity, and re-generation.

Objectives – Current study aims to identify potential Trk receptors agonist using *in-silico* screening and computational modeling, including binding affinity assessment and molecular dynamics simulations. The compound will be evaluated for neuroprotective effects in MPTP-induced SH-SY5Y and H₂O₂-induced N27 *in-vitro* Parkinson's models. Further validation will be conducted using a *Drosophila* model. The research also seeks to uncover the underlying neuroprotective mechanisms driven by Trk receptor activation.

Methods – The study adopts a comprehensive, integrative pipeline, combining *in-silico* modeling, *in-vitro* validation, and *in-vivo* pharmacological assessment to evaluate the neuroprotective efficacy of 7,8-dihydroxyflavone (7,8-DHF), in PD. Utilizing high-precision tool; Schrödinger's Maestro, the extracellular domains of trka and trkb receptors were structurally optimized through homology modeling, receptor grid generation, and molecular docking. Protein-ligand complexes were further refined using MM-PBSA and MD simulations. Parallel docking studies on D1 and D2 receptors enabled a dual-targeted therapeutic approach addressing both neuro-restorative and symptomatic dimensions. Mechanistic effects of 7,8-DHF were validated using SH-SY5Y and N27 dopaminergic neuronal cell lines subjected to MPTP & H₂O₂, evaluating mitochondrial dysfunction, apoptosis, and oxidative. Further, the therapeutic relevance was explored using transgenic *Drosophila* model overexpressing A30P α -Syn where behavioral, survival, and biochemical parameters were assessed.

Results – 7,8-DHF, was evaluated using an integrated strategy, encompassing *in-silico* approach, and appropriate *in-vitro*, and *in-vivo* PD models. Molecular docking and MMGBSA analyses demonstrated strong binding affinity of 7,8-DHF to the IG2 domains of trka and trkb, with MD simulations confirming complex stability. In SH-SY5Y and N27 dopaminergic neuronal cell lines, 7,8-DHF attenuated MPTP and H₂O₂-induced toxicity, reduced apoptosis, and ROS production, and preserved mitochondrial membrane potential. Additionally, in



transgenic *Drosophila* PD model, 7,8-DHF improved survival rates, restored motor functions, and significantly reduced oxidative stress, while enhancing catalase and superoxide dismutase activities.

Conclusion –7,8-DHF stands out as promising neurotrophin mimetic by activating Trk-signaling, conferring neuroprotection, supporting neuronal survival, and mitigating oxidative stress in validated PD models. These findings align with the evidence that neurotrophic factor-based strategies hold potential to impede neurodegeneration, rather than merely alleviating symptoms. Future research should focus on optimizing the pharmacological properties of such molecules. Additionally, combination approaches that pair neurotrophin mimetics with existing symptomatic treatments may further enhance therapeutic outcomes.



PC-DD-022: A Hexagonal Approach of *In-Silico* Discovery of Natural HIF-1 α Mimetics for Diabetic Wound Repair

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Background:

Diabetes mellitus impairs wound healing by disrupting critical molecular pathways such as VEGF and Wnt/ β -Catenin, both regulated by HIF-1 α . However, HIF-1 α is rapidly degraded due to its interaction with VHL via the ubiquitin-proteasome pathway. Inhibiting the VHL:HIF-1 α protein-protein interaction (PPI) could stabilize HIF-1 α and enhance wound healing in diabetic conditions.

Aims & Objectives:

Currently, no marketed molecules specifically inhibit the VHL:HIF-1 α PPI. This study aims to identify natural compounds capable of disrupting this interaction using a novel in-silico approach.

Methods:

The VHL: HIF-1 α interaction was confirmed through STRING with a PPI score of 0.999. The structure of VHL (PDB ID: 4W9H) was validated via a Ramachandran plot. A pharmacophore model with two acceptor and one donor feature was generated using pharmacist based on 23 known VHL inhibitors. Zincpharmer screened 179,679 natural molecules matching the model. ADMET profiling using Lipinski's rule of five filtered the hits to 105,493 compounds. Molecular docking was conducted in three phases (HTVS, SP, XP) using Glide, followed by MM-GBSA for binding energy estimation. The top 10 molecules were selected for molecular dynamics (MD) simulations.

Results:

Out of 6.1 million compounds, 179,679 met pharmacophore criteria and were further refined through ADMET screening. Docking stages shortlisted the top 100 candidates, and MM-GBSA analysis identified the top 10 based on ΔG binding energy. MD simulations revealed two lead compounds—ZINC95754342 and ZINC04098745—with stable binding to the VHL protein.

Conclusion:

This comprehensive *in-silico* approach successfully identified natural compounds with the potential to inhibit VHL: HIF-1 α interaction, representing promising therapeutic leads for diabetic wound healing.

Keywords:

Diabetic wound healing, HIF-1 α , VHL, Protein-Protein Interaction, Pharmacophore modelling, Molecular docking, Natural compounds.



PC-DD-023: Identification of Novel Molecules for HSP 90 C-Terminal Domain using computational tools

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Background:

The HSP90 as an anti-cancer therapeutic target has been around for the past two decades, and most of the HSP90 inhibitors that have entered clinical trials have had dosing, induction of heat shock response (HSR) and toxicity issues bound at the ATP binding site located in the N-terminal domain (NTD). The identification of a secondary nucleotide binding site at the C-terminal domain (CTD) and the subsequent discovery of coumermycin antibiotic Novobiocin as a C-terminal domain inhibitor with antitumor activity without inducing HSR, which has been a liability for the NTD inhibitors, and this has led to the development of new molecules with better affinity than novobiocin. In this proposed study, we hypothesise to develop novel and efficient CTD inhibitors as anti-cancer agents.

Aims & Objectives:

Design novel molecules targeting the heat shock protein 90 C-Terminal Domain.

Methods:

Previously reported highly active Coumarin and Biphenyl core CTD inhibitors were collected to identify Novel scaffolds. Scaffold-hopping and bio-isosteric matching methods were implemented and identified 50 different scaffolds and checked for their synthetic feasibility, predicted their ADMET properties for their drug likeness, and then utilised QSAR modelling, molecular docking, dynamic simulations, and binding free energy calculations to study ligand-protein complex behaviour.



PC-DD-024: Machine Learning and Molecular Modelling of P2X7 Antagonists from Natural Products as Anticancer Agents

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Background: The P2X7 receptor, an ATP-gated ion channel, is a critical factor in the progression of cancer by facilitating tumour growth, metastasis, and immune evasion. It is a prospective target for the development of anticancer drugs due to its overactivation in the tumour microenvironment. Based on medicinal chemistry endeavours, P2X7 inhibitors does not attain clinical approval due to its suboptimal pharmacokinetic profiles. Hence identification of selective and drug-like P2X7 inhibitors remains a significant challenge in drug discovery.

Aims & Objectives: The aim of the study is to identification of natural product-based P2X7 inhibitors from COCONUT database (among 6,95,133 compounds) using extensive in-silico approach involving machine learning (ML), pharmacokinetic screening, molecular docking and dynamic simulations.

Methods: The compound library was curated and evaluated for bioactivity using machine learning models (Random Forest, SVM) trained on known P2X7 antagonists. The structure based virtual screening (HTVS, SP, XP) was conducted, ADME-Tox properties were assessed using qikprop and HOMO-LUMO calculations using Jaguar for analysing the electronic stability of ligands. The Top ranked candidates underwent for MD simulations and MM-PBSA binding free energy analysis to confirm binding stability and potential efficacy.

Results: Several natural products were identified with high predicted affinity for the P2X7 receptor, favourable ADME-Tox properties, and stable electronic features. Molecular dynamics simulations revealed that these compounds maintained stable interactions with the receptor's binding pocket over the simulation period, indicating good binding stability and potential bioactivity.

Conclusion: This computational pipeline effectively prioritized natural product-based P2X7 receptor antagonists with drug-like characteristics. The top candidates identified in this study provide a strong foundation for further preclinical evaluation towards therapeutic development of anticancer agents.

Keywords: P2X7 receptor antagonists; Machine learning; Molecular docking; ADME-Tox; Molecular dynamics, Natural products, Anticancer agents.



PC-DD-025: Design, molecular docking, and ADMET studies of furan azetidinone hybrids as antifungal agents.

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1. Background:

Recent developments have demonstrated that furan-based hybrids, like furan-based compounds, can interact with important cellular targets and fungal enzymes to disrupt vital functions in fungal infections. The potential of these hybrids to circumvent resistance mechanisms and offer safer, more potent antifungal treatments is being investigated in this study.

2. Aim & Objectives

- To design and carry out the molecular docking studies for novel furan derivatives with enhanced anti-fungal potential.
- To evaluate binding affinity of furan to the target enzymes of *Candida albicans* via in silico docking.

3. Methods

Fifteen novel furan-azetidinone hybrid compounds (K1–K15) were designed via rational approach. Molecular docking was performed using Schrödinger's Glide module targeting fungal proteins: Sterol-14 a demethylase (PDB ID: 1E9X), Oxysterol binding protein [Osh4] (PDB id :1ZHX) Mevalonate-5-diphosphate decarboxylase (1FI4), Glycolipid - 2a mannosyl transferase (1S4N) and other proteins. These targets are obtained from Protein Data Bank source. Binding affinity of analogues for the targets were studied. Following drug likeness of the compounds were predicted using qikprop.

4. Results

Molecular docking results range from 1.917 kcal/mol to 10.446 kcal/mol

1. K15 showed the strongest binding with:

1ZHX (Oxysterol binding protein [Osh4]): –10.446 kcal/mol; 1AI9: –6.056 kcal/mol;
1JU6: –4.987 kcal/mol

2. K8 had good binding with:

1ZHX (Oxysterol binding protein [Osh4]): –10.075 kcal/mol; 1AI9: –6.516 kcal/mol

3. K12 showed strong binding with:

1ZHX: –10.015 kcal/mol :1AI9: –6.524 kcal/mol

4.K14 and K10 also showed strong binding affinities against 1ZHX and 1AI9.

5. Conclusion

The computational and biological findings highlight k15 as potent antifungal candidates with notable efficacy against *Candida albicans*. Their strong binding affinity and low MIC values suggest their promise for further optimization as antifungal agents. So K15 may be considered as a lead compound for the enhancement of antifungal activity.

6. Key words

Furan derivatives, antifungal activity, in silico docking



PC-DD-026: Design, Synthesis, and Antidiabetic Evaluation of New Indole Incorporated Thiazolidin-4-one Derivatives

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Background:

Diabetes mellitus remains a major global health challenge due to its chronic complications and the side effects associated with long-term drug therapy. The antidiabetic potential of the two versatile scaffolds, indole and thiazolidinone, has been thoroughly investigated. Therefore, new indole incorporated thiazolidin-4-one derivatives were designed and synthesized to find better compounds that target α -amylase and α -glucosidase.

Aims & Objectives:

To design and synthesize new indole incorporated thiazolidin-4-one derivatives and to assess their antidiabetic and antioxidant activities by in-vitro methods.

Methods:

A series of new indole incorporated thiazolidin-4-one were synthesized via cyclization of Schiff bases derived from substituted indole-3-carboxaldehyde and anilines, followed by reaction with thioglycolic acid. Synthesized compounds were characterized using IR, ^1H NMR, and mass spectrometry. They were subjected to in-silico analysis against human α -glucosidase (PDB ID: 3TOP) and α -amylase (PDB ID: 1HNY). In-vitro alpha-glucosidase and alpha-amylase inhibition assays, as well as DPPH and nitric oxide radical scavenging assays, were performed to assess antidiabetic and antioxidant activities.

Results:

The molecular docking studies showed that compounds CIT 2, CIT 5, and CIT 6 displayed the highest docking scores in comparison with standard Pioglitazone. When compared to standard ascorbic acid, Compounds CIT 2, CIT5, CIT 6, and CIT 10 showed significant IC₅₀ values for antioxidant studies by DPPH and Nitric oxide assay. Compounds CIT 2 and CIT 6 not only showed dual inhibitory activity on both the target enzymes in comparison with standard pioglitazone, but also were found to possess significant antioxidant activity.

Conclusion:

Compounds CIT 2 and CIT 6 were found to be promising molecules as antidiabetic agents when compared to all other synthesized compounds. Hence, these compounds may be used as lead molecules for future synthesis as antidiabetic agents.

Keywords:

Indole, Thiazolidin-4-one, Molecular docking, Antidiabetic, Antioxidant



PC-DD-027: Discovery and Biological Profiling of N-Phenyl-4,5-Dibromo Pyrrole Derivatives as potential Inhibitors of bacterial DNA Gyrase B subunit

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Background: Tuberculosis (TB), a contagious respiratory disease, has affected millions of human beings and resulted in their fatalities. The emergence of bacterial resistance to existing therapeutic agents has become an urgent concern for the health care sector. According to the recent Global TB Report of the WHO, TB was the leading cause of death from a single infectious agent in 2022.

Aim: Bacterial DNA gyrase continues to be a key and important target in the development of novel antibacterial agents. As possible inhibitors of *DNA gyrase*, we developed and synthesized a series of fourteen new N-phenyl-4,5-dibromo-pyrrole hybrids with substituted 1,2,3-triazole and isoxazole moieties.

Methods: A series of novel N-Phenyl-4,5-Dibromo Pyrrole hybrids were designed, synthesized with a good yield. The structure of the title compounds was characterized by physicochemical and spectral investigation (FTIR, ¹H NMR, and ¹³C NMR). Then, *in-vitro* DNA gyrase inhibitory assay, antibacterial, and antitubercular activity was assessed for all compounds. In-silico molecular docking and molecular dynamics simulations were performed to understand the mode of interaction of compounds with the target enzyme.

Results: The results clearly showed that four compounds had outstanding DNA gyrase inhibitory activity: **11b** (IC₅₀ = 0.28 μm), **17b** (IC₅₀ = 0.43 μm), **11a** (IC₅₀ = 0.90 μm), and **17a** (IC₅₀ = 0.72 μm). Two compounds **11b** (MIC = 1.56 μg/ml) and **17b** (MIC = 3.125 μg/ml) also exhibited the excellent anti-tubercular activity. Further, A docking analysis of the DNA gyrase revealed that these two compounds 11b (dock score of -7.01) and 17b (dock score of -6.60) displayed interaction with two important amino acid residues, ARG136 and ASP73. The MD simulations further provided thermodynamic binding energy, RMSD, and RMSF for these two compounds.

Conclusion: In summary, our study offers important insights into the structure-activity connection and binding interactions of these novel N-phenyl-4,5-dibromopyrrolamide hybrids as potential inhibitors of DNA gyrase B.

Keywords: Tuberculosis, Bromopyrrole, Molecular docking, DNA gyrase, Antibacterial activity.



PC-DD-028: Design of potential Anti-mexa antibacterial peptide based on machine learning technology, molecular docking and dynamic simulations

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Background:

Antibiotic resistance has materialized as a serious global health challenge, rendering many conventional therapeutic options as ineffective. Natural antimicrobial peptides (amps), found in several organisms, present a promising alternate with broad spectrum activity and distinct mode of action. Synthetic amps are currently in research as new weapons to combat infections due to resistant variants of pathogens and also overcome the drawbacks posed by natural amps like shorter half-life and lack of activity in physiological concentrations.

Aims & Objectives:

Computer-aided design of amps has envisaged to deliver evidence on chemical features and bioactivity prediction of designed peptide sequence(s) for antimicrobial potential as leads prior to synthesis. Here, it was proposed to design a series of amps applying several in silico modules and also assess the probability of the designed leads for its antimicrobial potential via efflux pump inhibition.

Methods:

Peptides sequences were collected from two databases viz., APD3 and dpamp. The obtained sequences were functioned by Random Forest (rf) and Artificial Neural Network (ANN) peptide designed methods and the designed peptides were further assessed via CAMPR4 online software. Computational framework at three levels was further utilized for envisaging novel peptides and their antibacterial intensities based on deep forest architecture-dpamp. Besides, the hemolytic levels and half-life were also analyzed for prediction followed by physicochemical parameters investigations. The resulting peptide sequences were studied for binding interaction(s) through molecular docking on the proteins, mexa, mexb and mexab-oprm. One potential candidate was further assessed for molecular dynamic (MD) simulations.

Results:

Around 18,000 peptide sequences were assembled for the design process. Based on the hemolytic activity and prediction of half-life, nine designed sequences were examined for the crucial protein-peptide interaction. The peptide, 2ANN exhibited robust interactions with the active site during 100 nanoseconds of MD simulations.

Conclusion:

The justification for selecting peptide 2ANN as the best AMP candidate is supported by its prediction for strong antimicrobial efficacy against multiple bacterial strains, low hemolytic activity indicating safety via the use of robust computational design methodologies.

Keywords:

Amps, AMP database, Random Forest, Artificial Neural Network, Molecular docking, MD simulations



PC-DD-029: Computational Insights into Bioactive Metabolites from *Burkholderia stagnalis* as Potential Inhibitors of Glutathione S-Transferase (GST) in *Escherichia coli*
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Background: *Burkholderia spp.* Devote over 20% of their genomes to secondary metabolite biosynthetic gene clusters, siderophores, yielding antibiotics and signaling molecules that drive ecological fitness. Despite of rich biosynthetic potential, a substantial proportion of these metabolites remain cryptic. Glutathione S-transferase (GST) in *Escherichia coli* which is a key detoxification enzyme which has a role in mitigating oxidative stress and contributing to bacterial antibiotic tolerance. Therefore, bioactive metabolites from *Burkholderia stagnalis* were investigated as Potential GST inhibitors.

Aims & Objectives:

- Explore *Burkholderia*-derived secondary metabolites for antibacterial activity.
- Identify potent GST inhibitors through combined experimental extraction and in-silico screening.

Objectives (i–iv): (i) extract metabolites (ethyl acetate partitioning) and assign functional groups (FTIR); (ii) dereplicate constituents via GC-MS; (iii) predict ADME/toxicity in silico; (iv) dock selected ligands against E. Coli GST to prioritise hits.

Methods:

1. Isolation & screening: Rhizospheric soil (Western Ghats, India) serially diluted (10^{-4} – 10^{-6}); agar-overlay assay selected active isolate.
2. Extraction: Broth extracted twice with ethyl acetate (1:1), organic phase evaporated to dryness.
3. Biophysical characterisation: FTIR (Perkin Elmer) and GC-MS (He, 250 °C) with NIST library matching.
4. Molecular characterisation: 16S rRNA sequencing, BLAST, phylogeny (genbank acc. No. PV151462).
5. Computational workflow: ligand preparation (pubchem → openbabel); swissadme, protox-3.0, GUSAR LD₅₀; GST structure (PDB 1A0F) prepared in Discovery Studio; docking in autodock Vina (grid 57.37, –33.08, 58.29); MD simulation in imods.

Results: The isolated bacteria was identified as *Burkholderia stagnalis*, further the FTIR analysis of crude extract revealed the peak at 3352, 2177, 1637 cm⁻¹ indicated the presence of amines, nitriles and alkenes group. Further GC-MS identified 24 metabolites, where major one included cyclobutyl tridecyl phthalate, 4-tert-octylphenol and pentaerythritol. All Metabolites met Lipinski's rules, four advances to docking and toxicity test. Cyclobutyl tridecyl phthalate exhibited the strongest binding affinity (–8.7 kcal/mol), forming hydrogen bonds with Gly50, Lys35, Gln51, and a π -alkyl interaction with Phe113, outperforming meta-chlorambucil (–5.6 kcal/mol). Imods dynamics confirmed the stability of the complex, and toxicity prediction placed the compound in moderate toxicity Class 3–4 with an estimated oral LD₅₀ of approximately 677 mg/kg.

Conclusion: *Burkholderia stagnalis* yields chemically diverse metabolites; cyclobutyl tridecyl phthalate emerges as a promising GST inhibitor with favourable drug-likeness. These insights warrant purification, enzymatic assays and synergy tests with existing antibiotics to combat GST-mediated resistance.



Keywords: *Burkholderia stagnalis*; secondary metabolites; GC-MS; GST inhibition; molecular docking.



PC-DD-030: Design and Assessment of a Transformer-Based Model to Predict Chemical Structures from Relevant Molecular Properties

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Introduction:

Designing novel drug molecules often requires reverse-engineering molecular structures from desired physicochemical properties, which is traditionally time-consuming and expert-driven. Recent advances in Artificial Intelligence (AI) have enabled data-driven generation of molecular structures, particularly using sequence generation models such as Transformers.

Aim & Objective:

To develop and evaluate a Transformer-based neural network model capable of generating SMILES (Simplified Molecular Input Line Entry System) molecular structures from physicochemical descriptors.

Methods:

A curated dataset of ~40,000 molecules with known SMILES and 17 key molecular descriptors (e.g., molecular weight, hydrogen bond donors/acceptors, rotatable bonds, topological surface area, xlogp3) was used. SMILES strings were tokenized and padded for sequence modeling. Molecular descriptors were normalized using standard scaler. A custom Transformer-based sequence-to-sequence model was implemented in tensorflow, embedding descriptor vectors as context inputs to an autoregressive SMILES decoder. The model was trained using categorical cross-entropy loss with teacher forcing. Performance was evaluated on a held-out validation set using metrics including Exact Match Accuracy, Sequence Similarity, and Chemical Validity (using rdkit).

Results:

The trained Transformer achieved ~42% exact match accuracy, ~84% average sequence similarity, and >97% valid SMILES generation. The model demonstrated strong generalization from numerical descriptors to syntactically and chemically valid molecular structures, highlighting the viability of descriptor-to-SMILES generation. Tanimoto similarity with true molecules averaged 0.78, indicating reasonable structural fidelity.

Conclusion:

This Transformer-based model provides a promising AI framework to design or recover molecular structures from desired physicochemical profiles, potentially accelerating early-stage drug discovery and lead optimization.

Keywords:

SMILES generation, deep learning, chemoinformatics, molecular descriptors, transformer model, drug design, structure prediction



PC-DD-031: Computational design and study of pyrimidine analogues for Alzheimer's disease.

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Alzheimer's disease (AD) is a serious condition that leads to memory loss and cognitive problems caused by amyloid-beta plaques and tau protein tangles. Pyrimidine analogues are being explored as potential drugs because they can target various aspects of AD. Computational design techniques, such as 3D-QSAR, molecular docking, and molecular dynamics simulations, are crucial for enhancing these treatment options. To design and optimize novel pyrimidine-based therapeutic candidates through integrated computational approaches involving 3D-QSAR, molecular docking, and molecular dynamics simulations for enhanced biological activity and target binding efficacy. The objectives include performing 3D-QSAR studies on pyrimidine derivatives, conducting molecular docking studies to evaluate binding interactions, and running molecular dynamics simulations for top-ranked complexes. Using pyrimidine as a key structure, we created a molecule for study, utilizing 53 molecules with Chemdraw. The models were compared based on predictive ability and error metrics, and their precision was assessed using various indices. MD simulations were conducted to analyse protein-ligand interactions. The study's results showed that Kpls_molprint2d_4 was the best autoqsar model, with $R^2 = 0.8572$ and $Q^2 = 0.7577$. Molecular docking identified P596-0414 and G435-1135 as top binders for 4MYQ, and L741-0931 and F832-0751 for 1XN0. Molecular dynamics simulations confirmed the stable binding and strong non-bonded interactions of these ligands. The study aimed to evaluate the performance and stability of the designed pyrimidine-based molecule through various predictive metrics and simulations.

Keywords:

Pyrimidine nucleus, Auto QSAR, Machine learning, Molecular docking, Molecular simulation, Alzheimer's disease



PC-DD-032: Investigation of some novel combinations of furan derivatives as potential anticancer agents: An in silico computational study.

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Background

Cancer is one of leading disease which causes death, characterized by the uncontrolled growth and spread of abnormal cells in the body.

The furan nucleus is known for various pharmacological properties such as antibacterial, antifungal including anticancer activity, while the azetidinone nucleus (β -lactam ring) also exhibits significant biological activities such as antibacterial and anticancer properties.

Combining these two active moieties to form furan-azetidinone hybrids may enhance their anticancer activity due to possible synergistic effects.

Aim & Objectives

- To design some of hybrid novel furan derivatives with enhanced anticancer potential.
- To evaluate binding affinity to key proteins involved in cancer via in silico docking.

Methods

Fifteen furan- azetidinone derivative compounds (K1–K15) were designed. Molecular docking was performed using Schrödinger's Glide module software. The hybrid derivatives targeting the enzymes such as human placental aromatase, EGFR protein kinase, topoisomerase II was evaluated and docking score was obtained ADMET parameters were predicted using QikProp.

Results

Molecular docking was performed for furan-azetidinone derivative and human placental aromatase and a very good docking scores ranging from -5.1 to -9.3 kcal/mol was obtained and also with other protein also good docking score was obtained. Compound K5 (3-ethoxy-4-ydroxy-phenyl) derivative showed the highest docking score with human placental aromatase (-9.2 kcal/mol) and K10 (2,4-dichloro-phenyl) derivative showed strong binding with topoisomerase II (-8.4 kcal/mol) indicating a very good anticancer potency, but K10 (2,4-dichloro-phenyl) derivative in EGFR protein kinase (-6.0 kcal/mol) did not show very good docking score.

Conclusion

The computational and ADMET parameter study findings followed and in accordance with lipinski's rule highlight K10 (2,4-dichloro-phenyl) derivative and K5 (3-ethoxy-4-ydroxy-phenyl) derivative as potent anticancer candidates with notable efficacy against human placental aromatase and topoisomerase II respectively. Their strong binding affinity values suggest their promise for further optimization as anticancer agents and development of hybrid derivative compounds.

Keywords

Furan derivatives, Azetidinone, hybrid derivatives, in silico docking, anti-cancer activity.



PC-DD-033: Synthesis and antimicrobial activity of novel pyrazine-linked 1,3,4-oxadiazole derivatives.

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Background:

The rise of multidrug-resistant pathogens poses a serious global health threat, necessitating development of novel antimicrobial agents. Combining the structural and pharmacological characteristics of Pyrazine and 1,3,4-oxadiazole provides a new and promising approach for developing dual-functional antimicrobial agents with enhanced efficacy and reduced potential for resistance by targeting multiple bacterial pathways.

Aims & Objectives:

To design and synthesize Novel Pyrazine-linked 1,3,4-oxadiazole derivatives and evaluate *In-vitro* antimicrobial activity.

Methods:

Novel Pyrazine-linked 1,3,4-oxadiazole derivatives were synthesized via cyclization of Pyrazine carbohydrazide with Carbon disulfide and Potassium hydroxide in alcohol solution, followed by reaction with α -chloro acetanilide. Synthesized compounds were characterized using FT-IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, HR-MS. These were subjected to *in-silico* studies including Molecular Docking, ADMET, MM-GBSA analysis and MD simulations. Anti-bacterial activity was assessed using Mueller Hinton Broth dilution method and anti-fungal activity using Sabouraud agar medium. Cytotoxic activity was evaluated using the MTT assay method.

Results:

Molecular docking studies showed that Compound A4 and Compound A8 exhibited docking scores comparable to standard Ciprofloxacin while Compound A3 and A1 demonstrated superior binding affinity against fungal targets, comparing to Ketoconazole. ADMET predictions suggested favorable pharmacokinetics and toxicity. MM-GBSA calculations indicated a favorable free binding energy. The compounds A7, A4, A3, and A1 possessed excellent antibacterial activity whereas compounds A1, A2, A3, A4, A5, and A8 possessed excellent antifungal activity when compared to standard Ciprofloxacin and Ketoconazole respectively. To ensure stability, 200 ns Molecular Dynamics simulations were conducted on the 4DUH-compound A4 complex. Cytotoxicity of the compounds performed on NIH3T3 cell lines were found to be non-toxic in nature.

Conclusion:

Compounds A1 and A3 emerged as the most effective, demonstrating potent antibacterial and antifungal activity. These molecules could serve as lead compounds for the development of next-generation antimicrobial agents.

Keywords:

1,3,4-Oxadiazoles, Pyrazine, Molecular hybridization, *In silico* analysis, antimicrobial activity, Cytotoxicity



PC-DD-034: Assessment of Anti-Asthmatic Potential of Bioactive Compounds from *Ficus religiosa* Using Computational Modeling and Mast Cell Stabilization Assay.

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Background:

Asthma is a chronic inflammatory airway disease affecting millions globally, with India contributing significantly to asthma-related deaths. Conventional treatments often cause side effects, prompting interest in safer alternatives. *Ficus religiosa*, a medicinal plant widely used in traditional Indian medicine, is known for its anti-inflammatory, antioxidant, and bronchodilatory properties. Hence, this study aims to conduct in-depth research on the bioactives of *Ficus religiosa* using various computational tools.

Aims & Objectives:

Aim: To identify a bioactive compound from the *Ficus religiosa* plant, responsible for anti-asthma properties, using computational analysis and the mast cell degranulation technique.

Objectives:

To identify the bioactive constituents of *Ficus religiosa* with therapeutic potential against asthma by target prediction methods

To evaluate the interaction and dynamic behavior of bioactive compounds from *Ficus religiosa* with key asthma proteins through molecular docking, molecular dynamics, and principal component analysis.

To validate the anti-inflammatory effects of selected *Ficus religiosa* compounds on mast cell degranulation in vitro.

Methods:

Bioactive compounds from *Ficus religiosa* were identified through the various data sources. Ligand and disease-related targets were predicted using Swiss Target Prediction and disgenet. PPI network identified the hub genes. Molecular docking studies evaluated the binding affinity with asthma proteins. Gene Ontology and KEGG pathway analyses were performed to understand the biological functions. Molecular dynamics simulations combined with MMPBSA, PCA, and FEL analyzed the stability and dynamics of top compound-target complexes. Finally, in vitro mast cell degranulation assays validated the anti-inflammatory effects of selected bioactives by measuring the inhibition of inflammatory mediator release.

Results:

Rutin from *Ficus religiosa* was identified as a key bioactive targeting asthma-related protein. Network pharmacology revealed the top 10 hub proteins involved in inflammatory pathways. Molecular docking showed strong binding affinities between rutin and targets such as phosphodiesterase 4D (PDE4D). Molecular dynamics simulations confirmed the stability of the rutin-PDE4D complex, supported by consistent RMSD and hydrogen bond interactions. In vitro mast cell degranulation assays demonstrated that rutin significantly inhibited the release of histamine and other inflammatory mediators, confirming its anti-inflammatory potential in asthma management.

Conclusion:

Rutin from *Ficus religiosa* shows promising anti-asthmatic potential by targeting key inflammatory proteins and inhibiting mast cell-mediated inflammation.

Keywords: *Ficus religiosa*, Asthma, Network Pharmacology, Molecular docking Simulation.

PC-DD-035: Isolation of phytoconstituents from root extract of *Bauhinia variegata* Linn and its antioxidant activity.

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Background: *Bauhinia variegata* Linn, a medicinal plant rich in secondary metabolites like flavonoids and phenolics, has been widely used in traditional medicine for its therapeutic properties.

Aims & Objectives: The present study involves the Isolation of phytoconstituent from root extract of *Bauhinia variegata* Linn and its antioxidant activity.

Methods: The general method involved collecting and authenticating the roots of *Bauhinia variegata* Linn, followed by shade drying, grinding, and Soxhlet extraction using petroleum ether and 90% ethanol. The extracts were concentrated using a water bath. Preliminary phytochemical screening was conducted to identify bioactive compounds. Antioxidant activity was evaluated using DPPH and TBA methods. Further, TLC and flash chromatography was employed for isolation of phytoconstituents. The isolated compounds are characterized by UV, IR, NMR, and Mass spectrometry and its antioxidant potential was assessed using the DPPH assay.

Results: The study revealed that the ethanolic root extract of *Bauhinia variegata* Linn exhibited significant antioxidant activity. Phytochemical screening confirmed the presence of carbohydrates, alkaloids, tannins, and flavonoids. In DPPH and TBA assays, the extract showed good free radical scavenging activity, with inhibition rates comparable to standards like ascorbic acid and BHT. Flash chromatography and spectral studies (UV, IR, NMR, and MS) confirmed the isolation of phytoconstituents such as quercetin, rutin, and flavonones. The isolated compound also demonstrated strong antioxidant potential, indicating that *Bauhinia variegata* Linn could be a promising source of natural antioxidants for therapeutic applications.

Conclusion: The ethanolic root extract of *Bauhinia variegata* and its isolated phytoconstituents exhibited strong in vitro antioxidant activity using DPPH and TBA assays. Spectral analysis indicated the presence of steroidal or triterpenoid compounds. These findings suggest potential therapeutic applications in treating oxidative stress-related diseases like cancer, inflammation, and aging.

Keywords: extraction, DPPH assay, TBA method, Antioxidant activity.



PC-DD-036: Synthesis, characterization, antimicrobial activity, and molecular docking studies of 1,5-diphenyl-1,2,4-triazole derivatives.

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Background: Bacterial infections cause significant mortality, particularly in hospitalized patients and developing nations. Diseases like tuberculosis, pertussis, and typhoid account for millions of deaths globally, highlighting bacteria's severe impact on public health.

Aims & Objectives: The present study involves the synthesis of new 1,2,4- Triazole derivatives and determining their antimicrobial activity.

Methods: Synthesis involves condensation reaction between aniline and substituted benzaldehyde to create a Schiff base, which was then cyclized with urea and zinc chloride to create 1,5-diphenyl-1,2,4-Triazole derivatives. IR and NMR spectroscopy were used for structure elucidation. Gram-positive and Gram-negative bacteria (*S. Aureus*, *S. Epidermidis*, *E. Coli*, *S. Typhi*) and fungus (*C. Albicans*, *A. Niger*) were used to test the compounds' antibacterial activity. Pyrx and Biovia Discovery Studio were used to perform molecular docking against *Candida albicans* Sterol 14- α demethylase (PDB ID: 5TZ1). The protein was obtained from RCSB PDB database.

Results: The synthesized compound were characterized by physicochemical and spectral data. Three compounds exhibited very good antibacterial activity on *Salmonella typhi* and *S.aureus* whereas no inhibition was observed on *S.epidermidis* and *E.coli*. The synthesized drugs also showed excellent antifungal activity on *Candida albicans* whereas none of the microbial inhibitory effect was observed in *Aspergillus niger*. Molecular docking studies revealed strong interactions with binding affinities ranging from -7.4 to -8.0, were methoxy derivative exhibited the highest interaction, with a binding score of -8.0.

Conclusion: This research involved synthesis and characterization of 1,5-diphenyl-1,2-dihydro-3H-1,2,4-triazole-3-one derivatives. Purity of compounds was confirmed by TLC and melting point, while IR and NMR spectroscopy were used for structure elucidation. Subsequently, antimicrobial activity was evaluated by determining minimum inhibitory concentrations (MIC) and zone of inhibition against various bacterial and fungal strains. Three out of seven synthesized compounds demonstrated significant antimicrobial properties, suggesting their potential as antibacterial and antifungal agents.

Keywords: Schiff base, 1,2,4-triazole, Anti-Microbial activity.



PC-DD-037: In silico study of binding affinities of novel small molecules against wild-type and mutant mmp13 and its impact on antitubercular activity

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Background:

Tuberculosis (TB) an infectious disease caused by *Mycobacterium tuberculosis* is posing serious challenges worldwide to control due to the emergence of drug-resistant strains. Existing therapies are not failing necessitating the need for the development of new antitubercular drugs that act through the inhibition of novel targets. Mycobacterial membrane protein Large 3 (mmp13) is one of the novel and promising target for antitubercular drug development. Mmp13 helps in transporting mycolic acids in the form of trehalose monomycolate across the cell membrane for mycobacterial cell-wall biosynthesis. Inhibition of this enzyme can result in the disruption of the cell wall biosynthesis leading to cell death. Mutations in the mmp13 gene have been reported and this can lead to drug resistance, particularly to those class of drugs that target mmp13.

Aims & Objectives: This study aims at analysing the in-silico binding affinities of small molecules in wild type and mutant mmp13 strains and identify the key interactions that are essential for molecules to exhibit activity against *Mycobacterium tuberculosis* bearing mutant mmp13 strains.

Methods: Reported small molecules with known antitubercular activity were retrieved from a recently published research article. After ligand preparation, ADMET property prediction was done using Qikprop tool. Homology models for mmp13 mutants were generated and protein reliability reports for the models were generated. The molecular docking studies against wild-type and mutant type mmp13 proteins were performed using XP docking protocol. Further Induced Fit Docking studies (20 poses generated for each molecule) was performed and the binding free energy of the complex was assessed through MMGBSA analysis. Molecular dynamic studies of the compounds were carried out for 100ns to study the stability of drug-target interactions.

Results: Significant differences in binding affinities of molecules were observed when compared to interaction with wild-type and mutant mmp13 proteins. Some mutations resulted in reduced binding efficiency, correlating with potential resistance.

Conclusion: This study provides insight into the structural and functional impact of mmp13 mutations on drug binding. The findings may guide the rational design of new inhibitors that retain efficacy against resistant *M. Tuberculosis* strains and support the use of *in silico* methods in preclinical drug evaluation.

Keywords: *Mycobacterium tuberculosis*, mmp13, Drug resistance, Binding affinity, Molecular Dynamic Study, MMGBSA, Induced Fit Docking



PC-DD-038: Exploring the therapeutic potential of Azetidinone derivatives: design, synthesis, and biological evaluation.

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Background: The development of resistance to antibacterial agents is increasing in recent years, particularly with pathogens such as MRSA and CRE posing major health threats. There is a need for the novel drug discovery. Azetidinone (β -lactams) and their conjugation with pharmacophores like pyrimidines may lead to enhanced antibacterial activity with great therapeutic importance.

Aim and objective: To design and synthesis of azetidinone derivatives tethered with pyrimidines and evaluate for antibacterial activity.

Methodology: A series of azetidinone derivatives were synthesized via a multi-step process involving the formation of Schiff bases and subsequent cyclization to obtain azetidinone derivatives tethered with pyrimidines. Some compounds were synthesized using microwave-assisted organic synthesis (MAOS) to enhance yield and efficiency. The synthesized compounds were characterized by melting point, ^1H NMR, and mass spectral analysis. Antibacterial activity was evaluated using the cup plate method and well diffusion technique.

Results: Some of the synthesized compounds exhibited antibacterial activity. Among these compounds, JPM1 (4-methyl derivative) showed promising antibacterial activity with a well-defined zone of inhibition using the cup plate method against *Staphylococcus aureus*, as compared to the standard ciprofloxacin and DMSO as the control. The formation of azetidinone derivatives was confirmed by spectral analysis using IR and NMR. The biological evaluation exhibited significant results against *Staphylococcus aureus*, with a clear zone of inhibition; however, the inhibition was slightly less than that of the standard ciprofloxacin.

Conclusion: The study identified compound JPM1 (4- methyl derivative) as a lead molecule with significant antibacterial potential. The combination of azetidinone tethered with pyrimidine pharmacophores serve as a valuable strategy in developing new antibacterial agents.

Keywords: Azetidinone, Pyrimidine, Synthesis, Antibacterial activity



PC-DD-039: In Silico Evaluation of Ginger (*Zingiber officinale*) Phytochemicals as Potential Inhibitors of dnak (Hsp70) Chaperone in *Escherichia coli*.

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Background:

Heat shock proteins (HSPs), particularly Hsp70 (DnaK in *E. coli*), are ATP-dependent chaperones essential for protein folding and survival under stress. Inhibiting DnaK can disrupt bacterial stress tolerance and virulence, making it a promising antibacterial target.

Aims & Objectives:

This study aims to explore the inhibitory potential of phytochemicals derived from *Zingiber officinale* (Ginger) against *E. coli* DnaK through in silico molecular docking, ADME analysis, and toxicity prediction.

Methods:

Ginger root extracts were obtained using Soxhlet extraction with methanol. GC-MS analysis identified 70 phytochemicals, of which 30 compounds met Lipinski's and Veber's criteria. Drug-likeness and ADMET properties were assessed using SwissADME and ProTox-II tools. Molecular docking of selected phytochemicals was performed using AutoDock Vina (PyRx) against the DnaK structure (PDB ID: 2KHO), and protein binding pockets were identified using GlycanInsight. Ramachandran plot validated the 3D protein structure. Dynamics and stability of interactions were studied using the iMODS server.

Results:

Eight phytochemicals exhibited favorable drug-likeness and low toxicity (Class 4–5). Docking revealed that **1,6,10-Dodecatrien-3-ol** had the strongest binding affinity (−7.9 kcal/mol), forming stable hydrogen bonds with key DnaK residues. iMODS dynamics simulation confirmed the stability of the ligand-protein complex. The Ramachandran plot showed 90.6% of residues in the most favored regions, validating the model's quality.

Conclusion:

Phytochemicals from Ginger exhibit promising binding interactions with DnaK, supporting their potential as natural antibacterial agents. Further in vitro and in vivo studies are warranted to validate these findings.

Keywords:

Hsp70, DnaK, *Zingiber officinale*, molecular docking, antibacterial, ADMET, GC-MS



PC-DD-040: Synthesis and Evaluation of Benzimidazole Derivatives as α -Amylase Inhibitors: Enzyme Kinetics and *In-Silico* Approaches

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Background:

Alpha-amylase is a key enzyme involved in carbohydrate digestion and plays a significant role in postprandial hyperglycemia. Benzimidazole derivatives have shown diverse pharmacological properties, including potential enzyme inhibition.

Aims & Objectives:

This study aims to synthesize benzimidazole derivatives and evaluate their inhibitory activity against α -amylase using in-vitro and in-silico methods. Comparative kinetic studies were conducted with standard drug Acarbose

Methods:

A series of benzimidazole derivatives—BENZOLE, 2PBI, PHABA, TMOXY, DMOXY, and VNLN—were synthesized by condensing *o*-phenylenediamine with substituted aromatic acids and aldehydes. Structural characterization was performed using IR and ^1H NMR spectroscopy. In-vitro α -amylase inhibition was assessed via the DNSA method using UV-Visible spectrophotometry. IC_{50} values were calculated for all compounds. Enzyme kinetics were evaluated by determining V_{max} and K_m . In-silico docking studies with the AMY2B gene were performed to assess binding affinity, compared with Acarbose.

Results:

Among synthesized derivatives, PHABA exhibited the highest percentage inhibition (50%), while Acarbose showed 85.12%. IC_{50} values indicated that BENZOLE (119.2 μm) was comparable to Acarbose (76.33 μm). Kinetic studies revealed that the synthesized compounds act via non-competitive inhibition, whereas Acarbose is a competitive inhibitor. Docking studies showed DMOXY had a binding affinity of -7.7 kcal/mol, slightly lower than Acarbose (-8.1 kcal/mol).

Conclusion:

The synthesized benzimidazole derivatives demonstrated moderate inhibitory activity against α -amylase, with potential for further development. BENZOLE and DMOXY showed promising in-vitro and in-silico profiles, supporting their relevance as lead compounds.

Keywords:

Alpha-amylase, Benzimidazole, Acarbose, IC_{50} , Enzyme kinetics, In-silico docking



PC-DD-041: Should Cofactor Interactions Be Considered When Designing Inhibitors During Drug Discovery?

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Background:

InhA, the enoyl-ACP reductase from *Mycobacterium tuberculosis*, is a validated target for tuberculosis therapy. Many established inhibitors, such as isoniazid (INH), rely on interactions with the NAD(H) cofactor for their inhibitory activity. However, resistance and efficacy issues have highlighted the need to re-evaluate the role of cofactor interactions in the drug discovery process for InhA inhibitors.

Aims & Objectives:

This study aims to assess the significance of cofactor (NADH/NAD⁺) interactions in the design and development of novel InhA inhibitors. The objective is to determine whether considering cofactor binding enhances inhibitor potency, selectivity, and resistance.

Methods:

A comprehensive literature review was conducted, focusing on structural biology, enzymology, and medicinal chemistry studies of InhA inhibitors. Comparative analysis was performed between cofactor-dependent (e.g., INH-NAD adduct) and cofactor-independent (e.g., diazaborines) inhibitor classes. Key metrics included binding affinity, inhibitory mechanism, and susceptibility to resistance.

Results:

Findings indicate that cofactor interactions are central to the mechanism of many potent InhA inhibitors, contributing to slow-onset kinetics and high binding affinity. However, cofactor dependency can also introduce vulnerabilities to resistance, particularly when activation or binding is compromised. Recent advances in cofactor-independent inhibitors demonstrate that potent inhibition can be achieved without reliance on NAD(H), potentially circumventing common resistance mechanisms. Structural analyses reveal both approaches are viable, with distinct advantages and limitations.

Conclusion:

Cofactor interactions play a pivotal role in the efficacy of InhA inhibitors and should be carefully considered during drug discovery. Both cofactor-dependent and cofactor-independent strategies have merit; the optimal approach may depend on the specific resistance landscape and desired pharmacological profile.

Keywords:

InhA, cofactor, NADH, tuberculosis, drug discovery, inhibitor design, resistance, isoniazid, slow-onset inhibition



PC-DD-042: Evaluation of Some Novel Furan Derivatives as Potential Antibacterial Activity Against E. Coli: A Computational and Biological Approach

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1. Background

The increasing resistance among Gram-negative pathogens necessitates the development of new antibacterial agents. Furan, a five-membered heterocyclic compound, has shown broad pharmacological potential. Functionalizing the furan nucleus offers a promising strategy for targeting resistant bacteria such as *Escherichia coli* and *Pseudomonas aeruginosa*.

2. Aim & Objectives

Aim of the work was to develop and evaluate novel furan derivatives as potential antibacterial agents against E. Coli using computational and biological approaches.

- To design and synthesize novel furan derivatives with enhanced antibacterial potential.
- To evaluate binding affinity to key Gram-negative bacterial proteins via *in-silico* docking.
- To assess *in-vitro* antibacterial activity against E. Coli and P. Aeruginosa.

3. Methods

Furan-based compounds were synthesized and characterized using UV, FTIR, NMR, and Mass spectroscopy. Molecular docking was performed using Schrödinger's Glide module targeting bacterial enzymes: DNA gyrase (PDB ID: 1KZN), topoisomerase II (1IJJ), and β -lactamase (4FH2). ADMET parameters were predicted using qikprop. In vitro antibacterial screening was conducted using agar diffusion (zone of inhibition) and broth dilution (MIC) methods at a concentration of 100 μ g/ml, with ciprofloxacin as the reference drug.

4. Results

Docking scores ranged from -5.1 to -9.3 kcal/mol. Compound K7 (2-[3-Chloro-2-(3-methoxy-phenyl)-4-oxo-azetidin-1-yl]-4,5-diphenyl-furan-3-carboxylic acid ethyl amide) showed the highest docking score with DNA gyrase (-9.3 kcal/mol) and β -lactamase (-8.7 kcal/mol), while K5 (2-[3-Chloro-2-(3-ethoxy-4-hydroxy-phenyl)-4-oxo-azetidin-1-yl]-4,5-diphenyl-furan-3-carboxylic acid ethyl amide) showed strong binding with topoisomerase II (-8.4 kcal/mol). *In-vitro*, K7 exhibited a zone of inhibition of 22 mm against P. Aeruginosa and 20 mm against E. Coli, compared to 24 mm and 21 mm, respectively, for ciprofloxacin. K5 displayed inhibition zones of 19 mm (P. Aeruginosa) and 18 mm (E. Coli). Minimum inhibitory concentration (MIC) values for K7 were 12.5 μ g/ml (P. Aeruginosa) and 25 μ g/ml (E. Coli), indicating strong antibacterial potency.

5. Conclusion

The computational and biological findings highlight K7 and K5 as potent antibacterial candidates with notable efficacy against Gram-negative strains. Their strong binding affinity and low MIC values suggest their promise for further optimization as antibacterial agents.

6. Keywords

Furan derivatives, antibacterial activity, Gram-negative bacteria, *in-silico* docking, *in-vitro* assay, DNA gyrase, β -lactamase, MIC, zone of inhibition



PC-DD-043: Exploration of Phytochemicals from Ayurvedic Formulations for the Treatment of Parkinson's Disease Using *In Silico* Approaches.

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Background: Parkinson's disease (PD) is a progressive neurodegenerative disorder marked by dopaminergic neuronal loss in the substantia nigra, resulting in impaired motor coordination. Conventional pharmacological treatments offer symptomatic relief but fail to halt disease progression.

Aims & Objectives: This study aims to identify potential neuroprotective phytochemicals from traditional Ayurvedic polyherbal formulations (PHFs) — Manasamitra Vatakam, Valiya Sahacharadi Tailam, and Dhanwantaram Kuzhampu — using comprehensive *in silico* approaches.

Methods: Phytochemicals were retrieved from public databases including PubChem, IMPPAT, and Dr. Duke's database. A total of 6056 compounds were compiled, of which 751 met drug-likeness criteria based on ADME profiling and Lipinski's Rule of Five using SwissADME. SwissTargetPrediction and PASS Online were employed to predict potential protein targets. Polypharmacological networks were constructed using Cytoscape to analyze plant-phytochemical-target associations.

Results: Lead phytochemicals were further evaluated via molecular docking against Parkinson's disease-relevant protein targets such as MAO-B, AKT1, MAPK3, and VEGF, using BIOVIA Discovery Studio. Top-scoring ligands including Cedrusin, Spermine, Sesaminol, and Alpha-tocopherolquinone were subjected to molecular dynamics (MD) simulations (50–100 ns) to assess stability and binding interactions. RMSD, RMSF, and radius of gyration analyses indicated stable ligand-protein complexes, notably for Cedrusin for MAO-B and Spermine for AKT1. However, abnormally high fluctuations in some protein systems suggest simulation limitations or structural instability.

Conclusion: This *in silico* pipeline demonstrates the potential of Ayurvedic formulations as a source of multi-target phytochemicals for Parkinson's disease therapy. The findings support further *in vitro* and *in vivo* validation toward the development of safe, natural neuroprotective agents.

Keywords

Parkinson's disease; Ayurvedic formulations; polyherbal medicine; phytochemicals; molecular docking; molecular dynamics simulation; MAO-B; AKT1; neuroprotection; *in silico* drug discovery



**PC-DD-044: Exploring PROTAC-based strategy for mitigating WEE1 kinase in cancer:
An *in-silico* approach**

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Background:

Proteolysis Targeting Chimeras (protacs) have emerged as a novel therapeutic modality for targeted protein degradation, offering an alternative to conventional inhibitors. This study focuses on the *in-silico* design of PROTAC molecules targeting WEE1 Kinase and optimize their pharmacological properties and efficacy.

Aims & Objectives:

Key metrics, such as binding affinity, linker flexibility, and ternary complex stability, to be evaluated using advanced computational tools.

Methods:

Molecular docking, protein-protein docking, and molecular dynamics simulations.

Results:

Computational analyses identified several promising PROTAC candidates with favorable binding interactions to WEE1 Kinase and E3 ligase. Simulations demonstrated enhanced linker flexibility leading to stable ternary complexes, with qualitative improvements in degradation efficiency over baseline models. Docking scores indicated strong affinity, and dynamics runs confirmed structural stability under simulated physiological conditions.

Conclusion:

The *in-silico* approach successfully optimized PROTAC designs for WEE1 targeting, highlighting their potential as effective degraders in cancer therapy. These findings pave the way for experimental validation and further refinement of pharmacological profiles.

Keywords:

PROTAC, WEE1 Kinase, targeted degradation, *in-silico* design, molecular dynamics, ternary complex



PC-DD-045: Preliminary Evaluation of Nanodiamond as a Drug Carrier: Structural Integrity and Controlled Release Potential.

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Nanodiamond (ND), owing to its exceptional surface area, tunable surface chemistry, and biocompatibility, has garnered significant attention in recent years as a promising drug delivery vehicle. While its efficacy as a drug carrier has been explored in several biomedical applications, comprehensive pharmaceutical analyses remain relatively sparse. This study presents a preliminary investigation into the carrier potential of nanodiamonds, focusing on their structural integrity, purity, and drug-binding capability. The synthesized nanodiamonds were characterized using X-ray Diffraction (XRD) and Raman spectroscopy to confirm their crystalline purity and phase composition. Transmission Electron Microscopy (TEM) was employed to determine particle morphology and nanoscale dimensions, ensuring uniformity and appropriate size distribution favorable for biomedical interaction. To evaluate the drug carrier capacity, High-Performance Liquid Chromatography (HPLC) and complementary analytical techniques were utilized to assess drug adsorption and release kinetics. Results confirmed the high surface area and the presence of functional groups on the ND surface that facilitate drug molecule attachment without compromising the core diamond structure. The analytical outcomes demonstrated that nanodiamond can stably adsorb model pharmaceutical compounds and allow for controlled release, indicating its promise in targeted delivery systems. These findings establish a foundation for future in-depth pharmacokinetic and therapeutic studies and suggest that nanodiamond may serve as an effective and stable nanocarrier in advanced drug delivery applications. Further research is warranted to explore its full potential in clinical settings, including cytotoxicity, in vivo biocompatibility, and long-term stability under physiological conditions.

Keywords: Nanodiamond, XRD, TEM, Raman Spectroscopy, HPLC



PC-DD-046: Identification of potential hits for targeting *Helicobacter pylori* urease: An *in-silico* approach using pharmacophore modelling, molecular docking and molecular dynamics studies

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Background: *H. Pylori* is a Gram negative, microaerophilic bacteria that infects over 50% of the global population. A peculiar characteristic of *H. Pylori* is its production of the urease enzyme, which enables the organism to survive the acidic environment of the stomach. Inhibiting urease is hypothesized to be a promising therapeutic approach for the eradication of *H. Pylori*.

Aims & Objectives: To perform an *in-silico* study to identify potential hits for targeting *H. Pylori* urease

Methods: *H. Pylori* urease (PDB ID: 6ZJA) was prepared using Schrodinger Maestro. Compounds were screened from various databases using the CHEESE platform with 2- $\{[1-(3,5\text{-dimethylphenyl})-1H\text{-imidazol-2-yl}]sulfanyl\}$ -N-hydroxyacetamide (DJM), acetohydroxamic acid and 3-(3,5-dichloroanilino)-N-hydroxypropanamide as reference molecules. Ligands were prepared and screened through pharmacophore model followed by molecular docking (HTVS, SP, and XP), MMGBSA, and quikprop analysis. Top hits were validated using molecular dynamics.

Results: The molecular docking studies identified around 500 hits from acetohydroxamic acid, and about 2000 compounds from DJM and 3-(3,5-dichloroanilino)-N-hydroxypropanamide screening. From these, the top 10 compounds from each set were selected based on favorable docking scores, binding energy and ADME properties. Most of the selected compounds exhibited key interactions with the active site nickel ions, which is important for urease inhibition. Additionally, the compounds also showed hydrogen bonds, and hydrophobic contacts that disrupted urease activity. Molecular dynamics also confirmed the stability of the molecules. The best hits identified are SB1_3AJ_000003f04dd (docking score: -12.387, binding energy: -43.15), MCULE-8200121398 (docking score: -10.159, binding energy: -38.26) and SB1_3BJ_000001f609e (docking score: -11.220, binding energy: -46.40) from DJM, acetohydroxamic acid, and 3-(3,5-dichloroanilino)-N-hydroxypropanamide screening.

Conclusion: We obtained top 10 compounds from each screening with promising predicted urease inhibitory activity. An *in-vitro* urease inhibition assay will be necessary to validate the activity of these molecules before progressing to the pre-clinical evaluation.

Keywords: *H. Pylori*, urease inhibitors, pharmacophore modelling, molecular docking, molecular dynamics



PC-DD-047: *Insilico* screening and binding stability analysis of thiazole-coupled isoxazole moieties as an antidiabetic agent targeting PPARG

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Background:

Thiazole-linked isoxazoles were screened as potential anti-diabetic agents targeting ppar γ using molecular docking, ADME, and simulation tools. Lead compound C139 showed strong binding (-11.11 kcal/mol) and stability. Toxicity and biological activity assessments further supported its druggability, highlighting C139's therapeutic promise for diabetes mellitus management.

Aims & Objectives:

This study aims to identify thiazole-linked isoxazoles as novel therapeutic candidates for diabetes mellitus by targeting ppar γ .

Molecular docking of designed ligands, ADME and toxicity profiling, pharmacophore modeling, molecular dynamics simulations, and evaluating biological activity to validate compound C139's druggability and clinical potential.

Methods:

Designed ligands (C1–C210) were converted to 3D structures using chemdraw and ligprep. Receptor ppar γ (PDB ID: 5GTN) was validated via Ramachandran plots. Molecular docking was performed using Glide XP, assessing binding affinity. ADME and physicochemical profiling were conducted using qikprop. Pharmacophore models were generated via Phase, while PASS and protox 3.0 tools predicted biological activity and toxicity levels, confirming drug-likeness and safety of selected compounds.

Results:

Among 210 screened ligands, compound C139 exhibited the strongest binding affinity to ppar γ with a docking score of -11.11 kcal/mol, outperforming pioglitazone. ADME profiling revealed excellent oral absorption and bioavailability. Pharmacophore modeling indicated key aromatic ring features enhancing receptor interaction. PASS analysis predicted high antidiabetic activity ($P_a = 0.47$), while toxicity profiling via protox showed reduced toxicity ($LD_{50} = 3000$ mg/kg, Class V) compared to pioglitazone. Overall, C139 demonstrated superior drug-likeness, safety, and therapeutic potential as a novel antidiabetic candidate.

Conclusion:

Compound C139 demonstrated strong binding affinity, structural stability, and low toxicity in targeting ppar γ , outperforming pioglitazone in key molecular simulations. These findings highlight C139's potential as an antidiabetic agent. The in-silico approach significantly reduced time and cost, warranting further experimental validation for clinical applicability.

Keywords:

Anti-diabetic; Isoxazole; Thiazole; Molecular Docking; Molecular dynamic simulation; Peroxisome proliferator-activated receptor gamma.



PC-DD-048: Fighting Resistance with Intelligence: An AI-Driven Multi-Target Approach Towards Design of HIV Inhibitors

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Background:

Despite global strides in HIV management, over 40 million people still live with HIV, and drug resistance is on the rise, threatening decades of progress. The emergence of mutant strains resistant to standard therapies calls for next-generation solutions that are both intelligent and resilient.

Aims & Objectives:

To design and prioritize mutation-resilient, multi-target inhibitors against HIV using AI-driven generative models and structure-based virtual screening.

Methods:

High-quality crystal structures of wild-type and clinically relevant mutant forms of HIV enzymes were curated and aligned. Deep learning-based generative models and machine learning algorithms facilitated the design and optimization compounds across the HIV targets. Hit compounds were rigorously filtered and prioritized based on their multi-target engagement, pharmacological suitability, and mutation tolerance. Validation includes **comparative docking and interaction profiling**, confirming that lead compounds retain key contacts even in mutant enzyme forms.

Results:

This pipeline aims to deliver chemically diverse, mutation-resilient inhibitors capable of maintaining efficacy against resistant HIV strains.

Conclusion:

Our AI-integrated, multi-target design framework demonstrates potential to accelerate the discovery of anti-HIV agents capable of maintaining efficacy against evolving, drug-resistant viral strains, which offers a blueprint for adaptive therapeutic discovery in virology.

Keywords:

HIV, multi-target drug design, AI in drug discovery, deep learning, machine learning, protease, reverse transcriptase, integrase, drug resistance, generative models, virtual screening



PC-DD-049: Design and *in silico* evaluation of Phenoxy acetamide derivatives as potential antidiabetic agents.

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Objective: This study explores the interactions of phenoxy acetamide derivatives with AMP-activated protein kinase (AMPK), a critical enzyme in cellular metabolic regulation, with a specific focus on the diabetes-related AMPK pathway (PDB ID: 6C9F). The research aims to evaluate the anti-diabetic potential of these compounds as activators of the AMPK catalytic subunit.

Methods: The study employed molecular docking using the Glide module to assess the binding interactions of the compounds. Subsequently, an Absorption, Distribution, Metabolism, and Excretion (ADME) analysis was performed using Qikprop. The binding free energy was calculated using the Prime Molecular Mechanics Generalized Born Surface Area (MM-GBSA) method.

Results: Ten compounds exhibited notable binding affinity and interactions, including hydrogen bonds, pi-cation interactions, and halogen bonds, with key residues such as LYS143, ARG222, THR33, MET36, PRO127, TYR120, LYS126, ARG117, MET84, LYS163, ARG131, ARG223, VAL129, HIS150, ASN147, and ASP89 in the AMPK catalytic subunit (PDB ID: 6C9F). Among these, 3-chlorophenyl phenoxy acetamide (compound 5) displayed the highest XP-docking score of -5.22 kcal/mol, indicating robust binding potential. Prime MM-GBSA analysis further supported its strong binding affinity, with δ_{bind} (-97.78 kcal/mol), δ_{lipo} (-10.26 kcal/mol), and δ_{vdw} (-44.00 kcal/mol). The ligand consistently interacted with residues PRO127, MET84, ARG117, and TYR120.

Conclusion:

3-chlorophenyl phenoxy acetamide (compound 5), featuring functional groups such as a primary amine (NH), chlorine (Cl), nitro group (N), and oxygen (O), demonstrates significant potential as an AMPK activator. These findings suggest its promising role as an anti-diabetic agent, particularly for type II diabetes.

Keywords:

AMP-activated protein kinase (AMPK), molecular docking, MM-GBSA, ADME, type II diabetes, *Metformin*, anti-diabetic agents.



PC-DD-050: Optimizing Drug Solubility through Molecular Modelling and Simulation Techniques

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Background:

Improving drug solubility is a crucial challenge in pharmaceutical development, especially with poor water-soluble drugs. This research particularly focuses on optimizing the solubility of drugs using Schrodinger Material Science Suite. Though there are many advances in preparing Nanostructured Lipid Carriers (NLCs), there is a gap in identifying suitable excipients in formulation.

Aims & Objectives:

To optimize the solubility of poorly water-soluble drug by identifying suitable excipients for NLCs using the Schrodinger Material Science Suite.

Methods:

The study employs advanced molecular modelling and simulation techniques using the Schrodinger Material Science Suite, which involves screening of wide range of lipids that improve solubility and bioavailability of drugs. Data collection includes computational predictions of solubility behavior and molecular interactions. Key steps include solvent screening, lipid selection, and optimization of NLCs. The novelty lies in computational approach, by reducing the need of multiple experimental trials which are expensive.

Results:

The study identified promising lipids that can significantly improve the solubility and bioavailability of drug. The study not only gives us the insight on selecting the solvent but also on the formulation stability on incorporating the total formula of the preparation through molecular interactions between drug and excipients. These results show the potential of computational tools in optimizing drug solubility and formulation.

Conclusion:

The study involves computational tools in the early stage of pharmaceutical formulation, which contribute to more efficient and cost-effective research and development.

Keywords:

Drug solubility, molecular modelling, simulation techniques, Nanostructured Lipid Carriers, Schrodinger Material Science Suite



PC-DD-051: Screening of natural product database using computational tools for the identification of possible MMPL3 inhibitors.

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Background: The tuberculosis-causing bacterium *Mycobacterium tuberculosis* (Mtb) has a complex lipid-rich cell wall structure and is crucial for its survival and pathogenicity. Lipid-rich cell wall forms a low-permeability barrier that protects Mtb against most antimicrobial drugs. This is one of the many challenges facing TB drug development. Disruption of the cell wall structure can enhance the entry of drugs resulting in mycobacterial cell death. Mycobacterial membrane protein Large 3 (mmpL3) enzyme is a validated target that is required for transport of trehalose monomycolates (tmms) across the cell membrane for cell-wall biosynthesis. Inhibition of this enzyme can result in the disruption of the cell wall biosynthesis leading to cell death. Many natural products have shown promising antimycobacterial activity, including against drug-resistant strains. Natural compounds can be used as leads for developing new anti-TB drugs.

Aims & Objectives: To screen the natural product database for the identification of potential mmpL3 inhibitors using computational tools.

Methods: For the present study, IMPAAT (Indian Medicinal Plants, Phytochemistry And Therapeutics) database was selected and the compounds listed in the database were subjected to detailed computational studies using various modules of Schrodinger suite. The detailed ADMET profile of compounds were predicted. Cryo-EM structure of mmpL3 (PDB ID 7NVH) was used for performing detailed molecular docking studies to analyze the interactions exhibited by the natural products with the catalytic site residues of mmpL3. MMGBSA study was performed to assess the binding free energy of the complex. Further, molecular dynamic studies were carried out to study the stability of drug-receptor complex and the interactions throughout the simulation period.

Results: A total of 1335 molecules were selected from the IMPAAT database and used in the present study. After ligand preparation, ADMET property prediction was done using Qikprop tool. 265 molecules were selected for the molecular docking studies after eliminating those molecules with undesirable ADMET properties. Molecules exhibiting interactions with catalytic site residues ASP TYR 251-252 & 640-641 and high docking scores were shortlisted for Induced Fit Docking (IFD) studies. 45 molecules were used for IFD studies (20 poses generated for each molecule) and the binding free energy of the complex was assessed through MMGBSA analysis. At the end, top 27 molecules were selected for molecular dynamic studies. Ten molecules that exhibited stable interactions throughout simulation period were shortlisted for the invitro antitubercular activity.

Conclusion: Through detailed computational studies, the present study enabled us to identify 10 potential novel natural product-derived anti-*Mycobacterium tuberculosis* compounds.

Keywords: *Mycobacterium tuberculosis*, mmpL3, Natural products, Molecular Dynamic Study, MMGBSA, Induced Fit Docking



PC-DD-052: Synthesis of Boron-Tethered Curcumin Analogues as Cytotoxic Agents

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Background:

Boron tethered curcumin derivatives will be a promising strategy to enhance their anticancer activity and selectivity, offering improved cytotoxicity against cancer cells while minimizing toxicity to normal cells.

Aims & Objectives:

The study involves the synthesis of Boron-tethered ketones as a curcuminoids, their structural characterization using FTIR, NMR, and mass spectrometry, evaluation by in-vitro cytotoxicity against eight different cancer cell lines including two normal cell lines.

Methods:

Thirteen boron-tethered curcuminoids were synthesized via a condensation reaction using 4-piperidone derivatives and 4-formylboronic acid in acetic acid, then structurally characterized. The compounds were evaluated for cytotoxicity against eight cancerous (Capan-1, HCT-116, LN229, NCI-H460, MOLT-4, HL-60, K562, Z-138) and two non-cancerous cell lines (HEL 299 and PBMC).

Results:

Thirteen boron-tethered curcuminoids were evaluated for cytotoxicity, with compounds 3d, 3g, and 3h showing promising selectivity against cancer cell lines, while others like 3i–3m exhibited high cytotoxicity but low selectivity due to normal cell toxicity.

Conclusion:

Thirteen boron-tethered curcumin analogs (3a–3m) were synthesized, characterized, and evaluated for cytotoxicity against eight cancerous and two non-cancerous human cell lines. Compounds 3d, 3g, and 3h showed favorable selectivity, with 3g being the most potent against Capan-1 and LN229, although none surpassed the reference drug nocodazole, which exhibited significantly higher cytotoxicity toward cancer cells.

Keywords:

Boron, Curcuminoids, Cytotoxicity, Anti-cancer, In vitro.



PC-DD-053: Exploring Pyridine-chalcone hybrids as tubulin polymerase inhibitors: synthesis, structural characterization and molecular docking studies

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Breast cancer is a significant global health challenge. MCF-7 cells are a crucial *in vitro* model for estrogen receptor (ER)-positive breast cancer studies, offering insights into disease characteristics and treatment responses. Chalcones have emerged as potent anticancer compounds, demonstrating cytotoxicity and the ability to inhibit tubulin polymerization. Current research utilizes computational approaches, like molecular docking, to design safer, more effective chalcone inhibitors. The aim of this study was to synthesize and assess the anticancer activity of novel pyridine-based chalcones. The study used various methods to create and analyze new pyridine-based chalcones. It involved software like Chemdraw, Open Babel, and Schrodinger for *in silico* experiments to simulate drugs. Researchers synthesized proteins and ligands for molecular docking studies. The chemicals were made using a Claisen-Schmidt condensation reaction and purified. Structural characterization included TLC, IR, mass spectrometry, and NMR studies. The MTT assay was used to test cytotoxic activity against MCF-7 cell lines, and turbidimetric analysis evaluated tubulin polymerization inhibition. Pyridine chalcones were synthesized and characterized by melting point, yield, TLC, IR, MS, and NMR. Cytotoxicity ranged from 1.5 ± 0.7 to $26.2 \pm 3 \mu\text{m}$. Tubulin polymerization inhibition and docking studies confirmed tubulin as the target. A04 showed the best activity ($\text{IC}_{50} = 7.5 \mu\text{m}$, binding energy = -9.422 kcal/mol). The synthesized pyridine chalcones showed improved binding affinity and cytotoxic activity against MCF-7 cell lines, indicating that pyridine-containing chalcones could serve as promising candidates for cancer therapy.

Keywords: Pyridine chalcones, molecular docking, Claisen-Schmidt synthesis, Tubulin polymerase.



PC-DD-054: Formulation and development of Phytoconstituent-loaded Nanoemulgel: Unlocking therapeutic potential of *Wrightia tinctoria* through Network pharmacology, *in-silico* screening for Psoriasis

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Background: Psoriasis is a chronic autoimmune skin disorder characterized by hyperproliferation of keratinocytes and inflammatory cytokine release. Traditional medicinal plants such as *Wrightia tinctoria* have been used in skin ailments, including psoriasis, but lack systematic scientific validation.

Aim & Objective: A phytoconstituent-loaded nanoemulgel for psoriasis will be developed by identifying *Wrightia tinctoria* phytoconstituents via literature and databases, predicting psoriasis-related targets through network pharmacology, and validating key compound-target interactions using molecular docking. The nanoemulgel will be formulated, characterized physiochemically, and its anti-psoriatic efficacy evaluated in appropriate *in vitro* models.

Methodology: Phytoconstituents of *Wrightia tinctoria* were identified from the IMPPAT database and screened for drug-likeness. Psoriasis-associated genes were retrieved from genecards and OMIM. Common targets underwent GO and KEGG enrichment via shinygo, and protein-protein interaction networks were constructed using STRING and visualized in Cytoscape. Key targets were selected through molecular docking using autodock, with pharmacokinetic profiling via swissadme and admetlab. A nanoemulgel was formulated by homogenizing oil and aqueous phases, then incorporating the nanoemulsion into a Carbopol 934 gel base.

Results: A total of 147 overlapping genes were identified between the plant compounds and psoriasis-related targets. Enrichment analysis revealed involvement in immune regulation, cytokine signaling, and apoptotic pathways, particularly TNF, IL-17, and NF- κ B. Core genes such as TP53, BCL2, CASP3, IL6, and HSP90AA1 were highlighted. Molecular docking showed strong binding affinities (< -22.70 kcal/mol) between selected compounds (e.g., Quercetin, Rutin) and key targets. ADMET results indicated favorable safety and pharmacokinetic profiles.

Conclusion: This study substantiates the ethnopharmacological use of *Wrightia tinctoria* in psoriasis management by elucidating its multi-targeted mechanisms involving immunomodulatory and anti-inflammatory pathways. The integrative approach combining network pharmacology, molecular docking, and advanced formulation highlights its potential as a topical therapeutic candidate

Key Words

Psoriasis, *Wrightia tinctoria*, Network pharmacology, Molecular docking, Nanoemulgel



PC-DD-055: AI-driven Discovery of Natural Product Inhibitors Targeting Enoyl-ACP Reductase in Tuberculosis

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Background

Cancer is one of leading disease which causes death, characterized by the uncontrolled growth and spread of abnormal cells in the body.

The furan nucleus is known for various pharmacological properties such as antibacterial, antifungal including anticancer activity, while the azetidinone nucleus (β -lactam ring) also exhibits significant biological activities such as antibacterial and anticancer properties.

Combining these two active moieties to form furan-azetidinone hybrids may enhance their anticancer activity due to possible synergistic effects.

Aim & Objectives

To design some of hybrid novel furan derivatives with enhanced anticancer potential.

To evaluate binding affinity to key proteins involved in cancer via in silico docking.

Methods

Fifteen furan- azetidinone derivative compounds (K1–K15) were designed. Molecular docking was performed using Schrödinger's Glide module software. The hybrid derivatives targeting the enzymes such as human placental aromatase, EGFR protein kinase, topoisomerase II was evaluated and docking score was obtained ADMET parameters were predicted using QikProp.

Results

Molecular docking was performed for furan-azetidinone derivative and human placental aromatase and a very good docking scores ranging from -5.1 to -9.3 kcal/mol was obtained and also with other protein also good docking score was obtained. Compound K5 (3-ethoxy-4-ydroxy-phenyl) derivative showed the highest docking score with human placental aromatase (-9.2 kcal/mol) and K10 (2,4-dichloro-phenyl) derivative showed strong binding with topoisomerase II (-8.4 kcal/mol) indicating a very good anticancer potency, but K10 (2,4-dichloro-phenyl) derivative in EGFR protein kinase (-6.0 kcal/mol) did not show very good docking score.

Conclusion

The computational and ADMET parameter study findings followed and in accordance with lipinski's rule highlight K10 (2,4-dichloro-phenyl) derivative and K5 (3-ethoxy-4-ydroxy-phenyl) derivative as potent anticancer candidates with notable efficacy against human placental aromatase and topoisomerase II respectively. Their strong binding affinity values suggest their promise for further optimization as anticancer agents and development of hybrid derivative compounds.

Keywords: Furan derivatives, Azetidinone, hybrid derivatives, in silico docking, anti-cancer activity.



PC-DD-056: Molecular Memory Polymers: Design of Smart Therapeutics with Programmable Binding Affinity

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Aim: To create drug molecules that are capable of self-activation following a specific delay, dependent on their inherent chemical structure and degradation profile.

Objectives

- To create drug candidates possessing intrinsic time-delay mechanisms.
- To examine and verify delayed activation profiles under physiological conditions.
- To test the biological safety and potency of the released drug.

Methodology

Phase I: Design and Choice

- Time-dependent chemical linkers-containing prodrugs (e.g., hydrazone, ester, carbamate) will be designed for 1 to 24 hours' lag-phase activation.

Phase II: Synthesis and Identification

- Chosen molecules will be synthesized through routine organic methodology and identified by NMR, MS, and FTIR for purity and structure validation.

Phase III: Time-Dependent Drug Release Studies

- Each compound shall be incubated in buffer solutions, and the release of drugs shall be determined at intervals (0–24 h) by HPLC or UV-spectroscopy to validate time-based activation.

Phase IV: Cell Testing

- Delayed-release drugs shall be tested on RAW 264.7 and THP-1 cells.
- Cell safety prior to activation shall be evaluated using MTT assay.
- Post-release activity shall be examined by determining decrease in inflammatory markers (e.g., TNF- α , IL-6).
- Only molecules that are safe prior to activation and potent subsequent to release will be shortlisted.

Expected results

Selected molecules are predicted to exhibit delayed controlled activation with reduced early toxicity and potent biological activity following release. This substantiates the potential for single-dose, time-programmed pharmacologic action within clinical practice.

Conclusion

Molecular Time Capsules represent a promising solution towards autonomous drug scheduling, reducing the necessity for outside stimuli or repeated dosing. Their capacity to deliver active agents at the appropriate time provides new avenues for targeted, time-specific treatment.

Keywords

Time-delayed activation, molecular time capsules, kinetic prodrugs, controlled drug release, self-cleaving linkers, programmed therapeutics



PC-DD-057: Harnessing Artificial Intelligence in Drug Discovery for Neurodegenerative Diseases: Accelerating the Path from Bench to Bedside

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Background: Neurodegenerative diseases (nds) such as Alzheimer's disease, Parkinson's disease, Huntington's disease and amyotrophic lateral sclerosis etc., are a rising global health issue. These are characterized by progressive neuronal dysfunction with cognitive and motor decline that is irreversible. Globally more than 55 million people are affected by neurodegenerative diseases. It is estimated that the cases will reach 139 million by 2050. Most remain incurable with limited disease modifying therapies.

Aims & Objectives: This research investigates how useful is artificial intelligence (AI) in finding new drugs for nds. The study explores strategies to improve target identification, identification of drug candidates, lead optimization, and therapeutic repurposing, while decreasing development time, costs, and attrition rate, in the context of precision medicine.

Methods: Recent literature from 2019-2025 was systematically reviewed in this study to identify AI-based methodologies and tools utilized along the drug development continuum. Tools included alphafold2 for protein structure prediction, pandaomics for multi-omics-based target identification, deeppurpose for drug/ target interaction modeling, molecuLenet and deepchem for virtual screening, molecular property prediction, and QSAR modeling. Applications were also identified for de novo molecule generation, ADMET optimization, and analysis of real-world data sources.

Results: AI platforms have transformed neurodegenerative drug discovery significantly. Specifically, alphafold2 enabled high-accuracy 3D modeling of the critical proteins implicated in AD (TREM2, APOE, BACE1), and pandaomics and knowledge graphs enabled the discovery of novel AD and PD targets. Deeppurpose was able to predict compound-target interactions, and molecuLenet/Deep Chem supported functionality such as high-throughput screening and identifying toxicity predictions.

AI-enabled drug repurposing identified Candesartan as a potential treatment for early-stage Alzheimer's in under 2 years and for under \$2M vs. 12-15 years and \$1.5-2.6B, respectively, with drug discovery.

Overall, AI can shorten early drug research time by 2-4 years and reduce costs by 30-40%, but we have to address model generalizability, interpretability and regulatory approval challenges.

Conclusion: Artificial intelligence is increasingly becoming a major contributor to drug discovery for neurodegenerative disorders - improving accuracy, efficiency, and individualization of therapy design. Because of the large-scale adoption of AI tools and the growing ability to cooperate across disciplinary borders and construct a flexible governance approach, the potential to facilitate the development of new therapeutics is unprecedented in the opportunities for the patient in terms of time to market.

Keywords: Artificial Intelligence, Neurodegenerative Diseases, Drug Discovery, alphafold2, pandaomics, deeppurpose, molecuLenet, deepchem, Machine Learning, Deep Learning, Virtual Screening, Target Identification.



PC-DD-058: Exploring Novel Therapeutic Targets in *Pseudomonas aeruginosa*: A Multi-Dimensional Approach to Combat Antimicrobial Resistance.

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Background: *Pseudomonas Aeruginosa* is a gram-negative bacterium, shaped like a rod, it is aerobic in nature. It causes opportunistic infections in humans but unlike the opportunistic bacteria which are usually present in the body and attack when the hosts immune system is weakened, *pseudomonas aeruginosa* while attacking when the immune system is weakened, it is quite ineffective against a non-weakened immune system. Examples of its opportunistic nature is that *Pseudomonas aeruginosa* infects damaged skin, causing life-threatening sepsis. Despite this, *pseudomonas aeruginosa* is most well known for its immense resistance to antibiotics. *Pseudomonas aeruginosa* does not merely use one way to avoid antibiotics but rather, it uses multiple methods to dodge antibiotics, it adapts rapidly in various ways to multiple antibiotics. This is why it causes such a significant therapeutic challenge.

Aims & Objectives: Aim: the aim of this project is to determine various new targets for either drugs not used or as potential targets to be targeted by novel drugs.

Methods: Research was done into various protein, enzymes and other cell organelles or chemicals essential for the functioning of *pseudomonas aeruginosa* and many organelles were shortlisted as potential candidates for drug targeting, once the organelles were shortlisted then their structures were analyzed after obtaining the structures from PDB and if said organelles or chemicals were obtained from PDB if there were any molecules that they disabled in the human body then those substrates were also analyzed and using sites such as NCBI Blast, RCSB PDB, ChEMBL, HHblits/HHpred similar molecules were found. After similar molecules were found, docking was done using software's such as Schrödinger to test binding strength and molecules which can neutralize said important organelles in the bacteria thus disrupting bacterial infection.

Results: Around a grand total of ten potential drug targets were discovered in *pseudomonas aeruginosa* with 3 of them having some potential drugs already in the market which the bacteria may not have already gained resistance to, thus, multiple potential drug targets were found for *pseudomonas aeruginosa* and many organelles or biomolecules which it has, have been determined as non-suitable drug targets for *pseudomonas aeruginosa*.

Conclusion: *Pseudomonas aeruginosa* remains a formidable pathogen due to its remarkable antibiotic resistance and opportunistic nature, posing significant therapeutic challenges. This study aimed to identify novel drug targets by analysing essential proteins, enzymes, and biomolecules within *P. aeruginosa*. Using multiple bioinformatics databases and softwares, ten potential drug targets were identified, three of which may already have antibiotics that the bacteria has not developed a resistance to. Molecular docking studies further validated binding interactions, which shows promising candidates for future drug development.

Keywords:

Keywords: *Pseudomonas*, Infections, Antibiotics, Resistance, Novel, therapeutic, opportunistic, immune system, Drugs



PC-DD-059: Bioanalytical Method Development and validation of drugs used as antiepileptic and antipsychotic: a Interaction Study

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Aim:

To develop a bio-analytical method and validate for the simultaneous estimation of Carbamazepine and Olanzapine as per USFDA guidelines.

Methods:

The chromatographic separation was achieved by using Accucore C18, (50 x 4.6mm, 2.6 μ) column by applying gradient elution using the mobile phase A consist of 0.1% Formic acid in water as an aqueous phase and methanol as an Organic modifier in the following gradient: initial 10%B is maintained for 1 minute, 1 to 6minutes (10 to 95% B), held for 3 minutes, 9 to 9.5 minutes (90 to 10% B) and held at 10% for 2.5 minutes, detection was carried at the 270 nm by employing 0.4 ml/min flow rate. The separation of drugs from the human plasma was achieved using protein precipitation technique by methanol.

Results:

The retention time was found to be 5.34 min and 7.86 min for olanzapine and carbamazepine respectively. The developed method has the linearity range of 50-250 μ g/ml and 20-100 μ g/ml for carbamazepine and olanzapine respectively and the regression co-efficient (r^2) is 0.9 for the both drugs. Robustness and injectable reproducibility are evaluated for the method and found to be within the limit and the results were reproducible.

Conclusion:

Based on these results, conclude that the developed method was precise and accurate for the simultaneous estimation of carbamazepine and olanzapine. This method can be adopted for simultaneous estimation of drugs and will be helpful for *in-vivo* studies in future days & pharmacokinetics studies.

Keywords:

Carbamazepine and olanzapine, Human Plasma, Validation, Ultra Performance Liquid Chromatography.



PC-DD-060: Green Chemistry approaches in pharmaceutical synthesis

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Background: Parkinson's disease (PD) is a progressive neurodegenerative disorder characterized by the loss of dopaminergic neurons in the substantia nigra, leading to tremors, bradykinesia, and postural instability. Current treatments focus primarily on symptom management rather than disease modification. Kojic acid (KA), a natural metabolite produced by *Aspergillus oryzae*, has shown neuroprotective effects in Alzheimer's models but remains unexplored in PD. The zebrafish (*Danio rerio*), due to its genetic similarity to humans and well-characterized central nervous system, is a suitable model for PD studies.

Aims & Objectives: To investigate the neuroprotective potential of Kojic acid in a rotenone-induced zebrafish model of Parkinson's disease, with behavioral, biochemical, and histopathological assessments.

Methods: Zebrafish were divided into six groups: Normal, Positive control, Standard (Levodopa), and Kojic acid-treated (5, 10, and 20 mg/L). PD was induced using rotenone (5 µg/L). KA was administered for 28 days. Behavioral parameters were recorded using ANY-maze software. On day 29, fish were euthanized, and brains were harvested for histopathological and biochemical analyses, including AChE, SOD, Catalase, and Glutathione assays.

Results: The 10 mg/L KA-treated group demonstrated significantly improved locomotor activity and anxiety-related behavior compared to the positive control. Biochemical assays revealed improved antioxidant enzyme levels and reduced oxidative stress markers. Histopathological findings supported neuronal protection in the KA-treated brains.

Conclusion:

Kojic acid, particularly at 10 mg/L, exhibited promising neuroprotective effects in the zebrafish PD model, suggesting its potential as a therapeutic candidate for Parkinson's disease. Further investigations in higher models are warranted to confirm its efficacy and mechanism of action.

Keywords:

Parkinson's disease, Kojic acid, Zebrafish, Neuroprotection, Rotenone, Antioxidants



PC-DD-061: Artificial Intelligence-Driven Innovations in Oncology Drug Discovery: Transforming Traditional Pipelines and Enhancing Drug Design

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Background:

Oncology drug discovery remains a challenging and time-intensive process, with high attrition rates and prolonged development timelines. Traditional experimental methods are often insufficient to navigate the complexity of cancer biology. Artificial Intelligence (AI) offers innovative solutions by streamlining target identification, lead optimization, and preclinical assessment, accelerating drug development.

Aim and Objective:

This study aims to explore AI-driven innovations in oncology drug discovery, focusing on how machine learning (ML) and deep learning (DL) models enhance target prediction, compound screening, and molecular design, ultimately reducing development time and costs.

Methods:

A systematic analysis was conducted, reviewing current AI methodologies in oncology drug discovery, including neural networks for biomarker identification, reinforcement learning for molecular generation, and ML-based virtual screening techniques. Data sources included pubmed, Scopus, and recent clinical trial repositories.

Results:

AI-driven platforms demonstrated significant improvements in early-stage drug discovery, reducing candidate screening time by over 40% and increasing hit-to-lead conversion rates. Predictive modelling showed high accuracy in identifying novel oncological targets.

Conclusion:

AI technologies are transforming oncology drug pipelines, offering precision and efficiency previously unattainable through conventional methods.

Keywords: Artificial Intelligence, Oncology, Drug Discovery, Machine Learning, Deep Learning, Drug Design, Target Prediction



PC-DD-062: Theranostics: Merging Pharmaceutical Innovation with Therapeutic Precision in Personalized Medicine

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Background:

Theranostics, a merging of "therapy" and "diagnostics," is a novel concept in pharmaceutical science that marries disease-specific imaging with targeted treatment through the identical molecular platform. It is a pivotal leap forward in translational medicine by translating findings in the laboratory into patient-individualized therapeutic strategies, most notably in oncology. The expanding use of radiopharmaceuticals is revolutionizing the future of personalized medicine.

Aim:

To describe the idea and clinical applicability of theranostics.

To discuss pharmaceutical advances making theranostic agents possible.

To evaluate therapeutic efficacy and Indian application.

Methodology:

This research dwells on radiopharmaceuticals such as Gallium-68 (Ga-68) for PET imaging and Lutetium-177 (Lu-177) for radionuclide therapy. Their key clinical use involves PSMA-based theranostics in metastatic prostate cancer and DOTATATE-based therapy for neuroendocrine tumors. Global research evidence as well as evidence from Indian institutions like Tata Memorial Hospital and AIIMS underlines prevailing use patterns.

Results:

Theranostics enhances target specificity, lowers toxicity, and allows real-time monitoring of treatment. It improves survival rates and quality of life over conventional chemotherapy.

Conclusion:

Theranostics is a revolution in bridging pharmaceutical innovation with personalized, effective therapy. Its increasing application in Indian oncology is a step toward precision medicine and individualized care.

Keywords:

Theranostics, Radiopharmaceuticals, Translational Medicine, Personalized Therapy



PC-DD-063: Unlocking histone deacetylase inhibition with chalcone chemistry

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Background:

Chalcones, an eminent scaffold, is well recognized for its anticancer properties. Increase in epigenetic regulator enzyme histone deacetylases (hdacs) has exhibited the mechanism of tumour progression in cancer cells. The role of chalcone scaffold in the inhibition of hdacs has been explored over the years.

Aims & Objectives:

The aim is to investigate the research progression reported on HDAC inhibition exhibited by compounds with chalcone scaffold and evaluate its potential in medicinal chemistry.

Methods:

The articles were sourced from multiple databases such as SCOPUS, Google Scholar and pubmed using keywords “chalcone” and “HDAC”. According to the structural features the reports are classified into two main categories. First, HDAC inhibition shown by zinc chelation of carbonyl functional group of chalcone scaffold. Second, zinc chelation is shown by known zinc-binding groups such as hydroxamic acids and the chalcone scaffold enhances interaction with the target. In each category there are sub-divisions based on presence or absence of heterocycles, dual inhibition and any other modifications.

Results:

Primarily, chalcone compounds with hydroxyl (-OH) substituents have shown therapeutical relevance. Although, the inhibition of hdacs by chalcone scaffold metal chelation has been shown, it is found comparable or less effective than known zinc-binding groups such as hydroxamic acids and benzamides.

Conclusion:

Evaluation of these research work enhanced the understanding of the chalcone scaffold in the inhibition of HDAC enzyme and interpretation of its effect on cytotoxicity. Analysis of influence of substituents offered insight for structural optimization. Further research on the structural modification may reveal improved metal chelation and enhanced cytotoxicity.

Keywords:

A,β-unsaturation, Anticancer, Antitumor, Chalcone, Epigenetics, HDAC, Inhibitor



PC-DD-064: Utilization of precision medicine digital twins for drug discovery in Alzheimer's disease

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Background:

Alzheimer's disease (AD) is a complex neurodegenerative disorder with limited treatment options and high clinical trial failure rates. Its heterogeneous nature highlights the need for precision medicine approaches. Digital twins—virtual, patient-specific models using multi-omics, clinical, and lifestyle data—are emerging as innovative tools to simulate disease progression and predict therapeutic outcomes.

Aim and Objective:

This review explores how precision medicine digital twins can accelerate drug discovery in AD by enhancing target identification, biomarker discovery, and personalized therapy development.

Methods:

A systematic review of studies from 2015 to 2025 was conducted using pubmed, Scopus, and Web of Science, focusing on AI-driven digital twin technologies, multi-omics integration, and in silico drug testing.

Results:

Digital twin models incorporating genomic, proteomic, neuroimaging, and clinical data improve patient stratification and drug efficacy prediction. Machine learning within these frameworks enables simulation of disease trajectories and testing of drug candidates virtually, reducing development time and costs.

Conclusion:

Digital twins represent a transformative approach in AD drug discovery, enabling personalized interventions and improved clinical outcomes. Future work should focus on model standardization, real-time data integration, and clinical validation.

Keywords: Precision Medicine; Digital Twins; Alzheimer's Disease; Drug Discovery; Artificial Intelligence; In Silico Modelling.



PC-DD-065: Exploring Human Fatty Acid Synthase as a Target in Cancer Therapy through Structural Analysis and Structure Activity Relationship of Domain-Specific Inhibitors

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Background

Fatty acid synthase (FAS) is an enzyme involved in the biosynthesis of lipids in humans. Its upregulation is significantly observed in cancer cells due to the increased demand for lipids and rapid cell proliferation. Cancer cells rely heavily on fatty acid synthesis to support their growth and maintain malignant properties. Over the past two decades, FAS has emerged as a promising target for cancer therapy, as its inhibition can disrupt lipid biosynthesis and reduce cancer cell viability. Among the various FAS inhibitors developed, TVB-2640 is the only one that has progressed into clinical trials.

Aims and Objectives

This review aims to provide a comprehensive overview of the structure and function of various domains of the human fatty acid synthase enzyme along with their respective inhibitors. A particular focus is placed on exploring the structure–activity relationship (SAR) of inhibitors targeting each domain.

Results

The review discusses in detail the domain-specific inhibitors of FAS and how structural modifications influence their interaction with the enzyme. It highlights how specific changes to the inhibitor structures can improve their binding affinity and selectivity toward different FAS domains.

Conclusions

By emphasizing structure–activity relationships, this review offers valuable insights into the rational design of novel inhibitors. Such domain-specific and structurally optimized inhibitors have the potential to effectively target FAS in cancer cells, opening new avenues for cancer therapy.

Keywords:

Human fatty acid synthase, Malonyl Acyl transacylase, Ketoacyl synthase, Dehydratase, Ketoacyl reductase, Thioesterase, Enoyl Reductase



PC-DD-066: Design and synthesis of triazole-linked indirubin derivatives as GSK-3 β inhibitors

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Glycogen synthase kinase-3 beta (GSK-3 β) is a type of enzyme that affects many different functions inside cells. In cancer, it can either help or stop the growth of tumours, depending on the situation. When GSK-3 β is not working properly, it can lead to faster cell growth, spread of cancer to other parts of the body, and resistance to treatment. Because of this, it is seen as a possible target for new cancer treatments. The compounds were designed to fight cancer by targeting GSK-3 β and stopping its harmful effects on cell growth.

Aim & Objective:

In this study, indirubin-triazole derivatives were designed, synthesised and tested for cytotoxicity against eight human cancer cell lines.

Methods:

The derivatives were synthesised and characterized by melting point, IR, ¹H NMR, HRMS. The synthesised compounds were screened against several cancer cell lines and normal cells.

Result:

Compounds were tested on Capan-1, HCT-116, LN229, NCI-H460, Molt-4, HI-60, K562, Z138 cells and on HEL299, PBMC normal cells. Among the synthesized compounds, AM-20 exhibited the more potent cytotoxicity for brain cancer (LN229 cell line) with CC 50 value of 4.78 $\pm$ 0.056 μ M compared to the standard Etoposide with CC 50 value of 9.14 $\pm$ 1.01 μ M.

Conclusion:

Among the synthesised compounds AM-20 exhibited better activity compared to the standard Etoposide. Further studies are conducted to establish the activity of AM-20 against the LN229 cancer cell line.

Keywords: GSK-3 β , indirubin-triazole analogues, LN229, brain cancer.

Category 7

Pharmacy Practice and Clinical Pharmacy



PP-CP-001: Development of a Precision Temperature-Controlled Drug Storage System Using iot Technology

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Introduction: Temperature-sensitive medications like insulin, vaccines, and biologics must be stored between 2°C and 8°C to maintain efficacy. In rural and resource-limited areas, a lack of consistent refrigeration poses a major risk to the integrity of such drugs. This project proposes a smart, portable, and cost-effective iot-enabled drug storage system to bridge this gap.

Aim & Objectives:

- Develop and construct a compact and affordable storage unit utilizing sensors and microcontrollers for accurate temperature control.
- Incorporate iot technology to enable real-time temperature monitoring, notifications, and remote access through a mobile or web interface.
- Test the system for reliability by examining its thermal stability and effectiveness in preserving medications.

Methodology: The system employs an Arduino Uno microcontroller with a DHT11 sensor for continuous temperature monitoring. A Peltier module, controlled via a relay, activates cooling when the temperature exceeds 8°C and deactivates below 2°C. An LCD displays live temperature data, while a buzzer and optional ESP8266/Bluetooth module provide local and remote alerts. The components are enclosed within an insulated box to optimize energy efficiency.

Results: Experiments demonstrated that the system reliably maintained temperatures within the targeted 2°C–8°C range across different environmental conditions. The automated cooling and alert system allowed for prompt actions to ensure the safety of the medications. The potential for iot integration further improved monitoring and accessibility.

Discussion: This device offers a viable, scalable solution for preserving temperature-sensitive drugs in decentralized healthcare settings. Its portability, simplicity, and real-time alert system make it ideal for fieldwork, mobile clinics, and emergency supply chains.

Keywords: Cold chain, temperature-sensitive medicines, iot, pharmaceutical storage.



PP-CP-002: Impact of Clinical Pharmacist Interventions on Drug-Related Problems and Therapeutic Outcomes in a Multispecialty ICU: A Prospective Study

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Background:

ICU patients are highly susceptible to drug-related problems (drps) due to polypharmacy and organ impairment. Clinical pharmacists play a vital role in identifying and resolving these issues.

Aim & Objectives:

To assess the impact of pharmacist interventions on drps and therapeutic outcomes in ICU patients.

Methods:

A 3-month prospective study was conducted in a tertiary care ICU. Drps were identified using PCNE classification, and pharmacist interventions were documented. Outcomes such as intervention acceptance, DRP resolution, ICU stay, and ADE prevention were evaluated.

Results:

Among 112 ICU patients, 186 drps were identified. Common drps included dosing errors (34.4%) and drug interactions (28%). Of 172 interventions, 86.6% were accepted. Accepted interventions led to improved safety and a reduction in ICU stay (7.2 vs. 8.6 days).

Conclusion:

Clinical pharmacist interventions significantly improve medication safety and therapeutic outcomes in ICU settings.

Keywords:

Clinical pharmacist, ICU, drug-related problems, pharmacist intervention, therapeutic outcomes



PP-CP-003: Development of a tool to enhance perceptions and adherence in chronic diseases

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Background: Chronic diseases are physical or mental conditions lasting over three months and requiring ongoing care. The patients' lack of information about the condition, its symptoms, and treatment significance can lead to poor adherence and worsening disease severity. This study emphasizes that effective chronic disease management requires understanding patient's attitude toward the condition and offering appropriate education.

Aims & Objectives: To develop and implement a tool to enhance patients' perceptions and medication adherence in chronic diseases.

Methods: An extensive literature search was conducted using search engines and mesh terms to develop an intervention to improve perception and adherence in patients with hypertension (HTN), diabetes mellitus (DM), and rheumatoid arthritis (RA). Med-tags were designed to include diseases definitions, complications, and lifestyle modifications. Seals provided information on medication dosage frequency. The med-tags were validated by a team of eight experts, including professors, lecturers, postgraduate students, and a clinical pharmacist. Readability was validated using the Flesch Reading Ease. Information was validated by ensuring the quality of information of study materials, and the layout and design were validated using the BALD method.

Results: Readability was evaluated using the Flesch Reading Ease (FRE) score. The final FRE score was 64.0, indicating that the med-tag readability is "standard", suitable for 15 to 16 year-old students. The EQIP score was found to be 62.4%. A higher EQIP score ensures high quality of the information in the med-tags. The BALD assessment score was found to be 23, indicating a standard design and layout.

Conclusion: The med-tags designed to improve patient perceptions and medication adherence were developed and implemented. Such interventions highlight pharmacists' vital role in educating patients and influencing their perceptions and treatment adherence. Future studies should investigate med-tags for other conditions like asthma and tuberculosis.

Keywords: Perception, Adherence, Med-tags

PP-CP-004: SEDENT-DM Study: Sedentary Exposure and Diabetic Echocardiographic analysis in Type 2 Diabetes Mellitus: A Prospective Cohort Study

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Study Design

Prospective cohort study

Objective

To examine the associations between sedentary behavior patterns and cardiovascular-metabolic parameters in adults with Type 2 diabetes mellitus (T2DM).

Methods

Setting: This prospective cohort study was conducted at NIMS Hospital, Rajasthan, India, with baseline assessments and follow-up evaluations [add specific dates - month and year start to finish].

Participants: We enrolled 72 adults with established T2DM diagnosis. Eligibility criteria included confirmed T2DM diagnosis, age ≥ 18 years, and ability to provide informed consent. Participants were recruited through hospital diabetes clinics. Follow-up methods included structured clinical assessments and echocardiographic evaluations.

Variables: Primary outcomes were echocardiographic parameters indicating cardiac function: left ventricular end-diastolic volume (LVEDV), left ventricular end-systolic volume (LVESD), isovolumetric relaxation time (IVRT), and E/e' ratio. Primary exposures were daily sedentary time (lying and sitting duration) assessed via structured interviews.

Statistical Methods: Pearson correlation analysis and multiple linear regression models were employed to assess associations between sedentary behavior and cardiovascular parameters, controlling for potential confounders including age, gender, BMI, and diabetes duration.

Results

Participants: 72 participants completed baseline assessments with completing follow-up evaluations.

Main Results: Participants (mean age 52.82 ± 9.29 years, 61.1% male) demonstrated substantial sedentary behavior (lying: 8.06 ± 1.45 hours/day; sitting: 6.35 ± 2.27 hours/day). Mean BMI was 25.03 ± 3.84 kg/m², blood pressure 139.72/87.08 mmHg, and hba1c $6.56 \pm 1.71\%$. Cardiovascular disease history was present in 62.5%.

Increased lying time showed significant positive correlation with IVRT (correlation coefficient and 95% CI to be specified) and significant negative correlations with LVEDV, LVESD, and right atrial diameter ($p < 0.05$). Prolonged sitting time demonstrated positive correlation with E/e' lateral ratio and left ventricular end-diastolic diameter ($p < 0.05$), indicating progressive diastolic dysfunction.

Conclusions

Sedentary behavior patterns demonstrate independent associations with early cardiac dysfunction markers in T2DM patients, particularly affecting diastolic function. These findings suggest that targeted interventions addressing sedentary time reduction should be integrated into comprehensive diabetes management strategies.



Keywords: Type 2 diabetes mellitus; sedentary behavior; echocardiography; cardiovascular risk; diastolic dysfunction; prospective cohort study

PP-CP-005: The Impact of a Pharmacist-Led Educational Tool in Chronic Disease Management

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Background:

Medication non-adherence in chronic disease patients often stems from misperceptions about their illness and treatment. In India, where structured patient education is limited, pharmacist-led interventions using simple, informative tools can enhance illness perception and adherence, leading to better chronic disease management.

Aims & Objectives:

To evaluate the impact of a pharmacist-led educational intervention in improving illness perception and medication adherence among chronic disease patients.

Methods:

A prospective interventional study was conducted over 6 months at a tertiary care hospital in Southern India. Adults (≥ 18 years) with Hypertension, Diabetes Mellitus, and Rheumatoid Arthritis(RA) were enrolled. Illness perception and medication adherence were assessed at baseline using the Brief Illness Perception Questionnaire (BIPQ) and Morisky Medication Adherence Scale (MMAS-8). Participants received individualized counselling and an educational tool designed to improve disease and treatment understanding. After 60 days, follow-up assessments were conducted using the same questionnaires. A paired t-test compared pre- and post-intervention scores, evaluating the educational tool's effectiveness.

Results:

200 patients (52% male, 48% female) were enrolled. Baseline scores in key illness perception domains were low: Personal Control (~ 5.4), Treatment Control (~ 4.7), and Illness Understanding (~ 5.1). 60 days post-intervention, significant improvements were seen across these domains ($p < 0.05$) in all three disease groups. Emotional Response showed no significant change. Medication adherence scores improved significantly in patients with Hypertension (6.5 to 7.1, $p < 0.0001$) and Diabetes (6 to 6.7, $p < 0.0001$) and modestly in RA (6.5 to 6.7, $p = 0.0730$). The intervention improved illness perception and adherence, especially in hypertensive and diabetic patients.

Conclusion:

Pharmacist-led education significantly improved patient outcomes. In the future, pharmacists should set aside dedicated time for patient counselling using visual aids and written instructions. Such personalized attention can significantly enhance the patient experience, engagement, medication adherence and overall treatment success.

Keywords:

Pharmacist counselling, Educational tools, Medication adherence, Illness perception



PP-CP-006: A Randomized Controlled Trial on Desidustat for Anemia Management in Diabetic Kidney Disease

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Background & Objective: Anemia is a common and serious complication in patients with DKD, often leading to worsened clinical outcomes. While eses such as epoetin alpha are standard therapy, their limitations include cardiovascular risks, injection burden, and ESA resistance. Desidustat, a novel oral HIF-PHI, may offer a more convenient and physiologically beneficial alternative for anemia management in DKD. The objective of the study is to compare the efficacy, safety, and effects on iron metabolism and quality of life between desidustat and epoetin alpha in patients with DKD-associated anemia.

Methods: In this open-label, randomized, parallel-arm trial, 52 adults (aged 30–70 years) with DKD and anemia (Hb <11.5 g/dl) were allocated to receive either desidustat (50 mg orally every 2 days) or epoetin alpha (4000 IU subcutaneously once weekly) for 12 weeks. Primary and secondary outcomes included hemoglobin (Hb), iron parameters, renal function, inflammation (CRP), and quality of life (KDQOL questionnaire). Statistical analysis involved independent t-tests, with significance set at $p < 0.05$.

Results: At 12 weeks, both groups showed significant increases in hemoglobin: mean change was $+1.8 \pm 0.6$ g/dl in the desidustat group and $+1.7 \pm 0.7$ g/dl in the epoetin alpha group ($p = 0.62$, NS). The desidustat group showed significantly greater improvement in serum iron (mean increase: 19.5 ± 6.3 μ g/dl vs. 12.1 ± 5.4 μ g/dl, $p = 0.01$) and transferrin saturation (increase: $5.6 \pm 2.1\%$ vs. $3.1 \pm 1.9\%$, $p = 0.03$) compared to epoetin alpha. Ferritin reduction was more pronounced in the desidustat arm (-34.2 ± 14.7 ng/ml vs. -21.8 ± 13.5 ng/ml, $p = 0.04$). CRP levels decreased more substantially with desidustat (-2.8 ± 1.2 mg/L vs. -1.3 ± 1.0 mg/L, $p = 0.01$), suggesting greater anti-inflammatory effect. No significant differences were seen in renal function changes (serum creatinine or UACR, all $p > 0.05$). Quality of life scores (KDQOL) improved in both groups, with a greater improvement in the desidustat group (mean score increase: 16.3 ± 5.7 vs. 10.8 ± 5.2 , $p = 0.02$). Both drugs were well-tolerated, with mild adverse events and no significant difference in incidence ($p = 0.73$).

Conclusion: Desidustat demonstrated comparable efficacy to epoetin alpha in improving hemoglobin levels among DKD patients with anemia, with additional benefits in iron utilization, inflammation reduction, and quality of life. Its oral administration and favourable safety profile suggest desidustat may be a preferred alternative to injectable eses in this population.

Keywords: Desidustat, diabetic kidney disease, anemia, HIF prolyl hydroxylase inhibitor, randomized controlled trial, epoetin alpha.

PP-CP-007: Health-related quality of life in heart failure patients: A prospective study

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Background:

Heart failure is a clinical syndrome where the heart is not pumping enough blood when compared to normal circumstances. We aimed to ascertain the health-related quality of life among heart failure patients. Secondly, we wished to assess the knowledge, assessment, and practice of heart failure patients.

Aim:

In this study, we assessed the Health-Related Quality of Life in Heart Failure patients.

Materials and methods:

In this prospective study, 49 cases of Heart Failure were included. Data collected were coded in SPSS software for statistical analysis. The correlation between KAP and HRQOL was assessed with Pearson correlation. A P-value of $0f < 0.05$ was considered statistically significant

Results:

About 49 patients were included in the study. 78% of the population was male and 22% were female.

The patients had moderately to poor Health-Related Quality of Life in all domains. However, most of the patients had poor scores in the physical dimension. In this study assessing the knowledge of heart failure patients, only 4% of the patients had their knowledge graded well.

Conclusions:

The results of our study imply that patients have a moderately poor health-related quality of life overall and poor physical dimensional scores. HRQOL was found to have a direct positive relationship with Knowledge, Attitude, and Practice.

Key Words:

Health-related quality of life, Knowledge, attitude, practice



PP-CP-009: Effects of Diabetes Mellitus on Pulmonary Function: A Comparative Cross-Sectional Study on Ventilatory Defects

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Introduction: Diabetes mellitus (DM) has been linked with a wide range of complications that may involve several systems and organs. Recent studies suggests that lungs are found to be a target organ for diabetes mellitus due to their rich supply of capillaries. This study endeavours to analyse the influence of DM on pulmonary function in the light of ventilatory defects among diabetic subjects.

Aim & Objectives:

To assess the impact of DM on PFT using a plethysmograph and to identify the most prevalent ventilatory defect in diabetics by categorizing them based on ventilatory defect types and severities.

Methods:

A comparative cross-sectional study was conducted on diabetic and non-diabetic subjects. Data includes patient demographics, current health status, and spirometry results. Data was analysed using descriptive statistics and appropriate tests in SPSS.

Results:

Diabetic subjects showed a 2.8-fold increased risk of developing ventilatory defect compared to non-diabetics, with a notably higher prevalence of obstruction.

Conclusion:

This study highlights the connection between diabetes and respiratory health, revealing that diabetes can lead to ventilatory defects. Overall, a combined approach of diabetes management and regular pfts is essential for optimizing patient care.

Keywords:

Diabetes Mellitus (DM), Pulmonary Function Test (PFT), Spirometry



PP-CP-010: A Prospective Study on Prescription Pattern on Drugs Used in Polycystic Ovarian Syndrome and Its Multidimensional Impacts On Women's Health.

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Background:

Polycystic ovary syndrome (PCOS) is a common endocrine disorder that affects approximately 8%-13% of women of reproductive age worldwide. It is characterised by a range of symptoms, including hirsutism, acne, menstrual irregularities, and poses a significant psychological burden, including anxiety and depression.

Aims:

The purpose of the study is to assess the most commonly prescribed drugs in PCOS and to evaluate the multidimensional impacts of PCOS on women's health.

Method

Study design.

“PROSPECTIVE INTERVENTIONAL STUDY “

Data source:

- Patient profile from wards
- Prescription
- Data collection form

Result:

The study reveals that among women with polycystic ovarian syndrome (PCOS), symptoms related to **pain, discomfort, and menstrual abnormalities** are the most prevalent. A majority of patients experienced **abdominal bloating (69%), menstrual cramps (68%), and irregular cycles with heavy bleeding (67%)**, indicating significant menstrual and hormonal disturbances. Other commonly reported issues included **excessive body hair (54%), fatigue (53%), headaches (49%), depression (41%), obesity (23%), and infertility (23%)**, highlighting both physical and psychological impacts. To manage these symptoms, **hormonal medications** such as **Duphaston 10 mg, Letroz 2.5 mg, Crina NCR 15, and Traptic MF** were frequently prescribed.

Conclusion:

The study confirms that PCOS has a broad impact on women's health, with menstrual issues and hormonal imbalances being most common. Symptoms like hirsutism, fatigue, and infertility highlight its physical and emotional burden. Hormonal drugs are frequently used, emphasizing the need for a comprehensive, patient-focused treatment approach.

PP-CP-011: Comparing the effectiveness of medication adherence using the medisafe mobile application versus pillo mobile application in type 2 diabetes mellitus patients in the south indian population – a randomised controlled trial

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Introduction:

Diabetes mellitus, a chronic metabolic condition, is characterized by consistently high levels of blood sugar. Medication adherence plays a pivotal role in maintaining optimal glycaemic control in type 2 diabetes mellitus (t2dm), thereby preventing complications. Mobile health (mhealth) technologies are promising intervention in improving medication adherence among patients with t2dm. The aim of this study is to determine the effectiveness in medication adherence mobile applications compared to conventional counselling in improving the medication adherence among t2dm patients. This study aims to bridge the gaps due to lack of understanding the true potential by conducting a randomized controlled trial that will offer insights into the real-world applicability and benefits of medi-safe and pillo in south india.

Method:

This prospective study comprising of total of 120 t2dm patients were randomized to group a (n=40) t2dm patients using medi-safe application, group b(n=40) t2dm patients using pillo mobile application and group c (n=40) patients receiving general counselling. These patients were enrolled based on the inclusion and exclusion criteria. The assessment of medication adherence was done using medication adherence rating scale (mars) and the improvement in glycaemic parameters were noted at the baseline (initial visit) and at the follow up (3 months). Statistical analysis was done using ms excel and graphpad prism.

Results:

The study demonstrated significant increase ($p < 0.002$) in medication adherence with patients using medi-safe application compared to pillo app and standard treatment group. Glucose profile among 3 groups also showed notable difference over the study period. Google form was circulated among patients in which majority responded that medi-safe was easier to use than pillo.

Conclusion:

the patients who used mobile applications showed marked improvement in medication adherence than those who were given only standard counselling session. Incorporation of medi-safe and pillo app into diabetes care protocol not only increased patient outcome but also contributed to better glycaemic control.

Keywords:

T2dm, mhealth, medisafe, pillo



PP-CP-012: Comprehensive Assessment of Opportunistic Infections, Antiretroviral Therapy and Initiatives for Children and Adolescents Living with Human Immunodeficiency Virus at Support Centres in Dakshina Kannada”

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Background and Objective: In India, pediatric HIV/AIDS remains a concern; challenges persist despite government efforts, including opportunistic infections and ART access. This study aimed to determine opportunistic infection prevalence, evaluate government ART impact, and assess HIV/AIDS initiatives in Dakshina Kannada.

Materials and Methods: A cross-sectional study was conducted at comprehensive care centers for children and adolescents living with HIV/AIDS in the district. Data were collected through face-to-face interviews using a structured questionnaire, covering socio-demographics, health status, healthcare access, and support services. Convenient sampling was employed and data was analyzed. 35 children met the inclusion criteria from three support care centers and participated in the study.

Results and Discussion: Analyzing their response, it was observed that opportunistic infections were rare, with most children receiving treatment and preventive care. All children were on ART, predominantly Tenofovir, Lamivudine, and Dolutegravir, with high adherence rates and reported side effects. Government initiatives were somewhat effective, but challenges persisted, particularly in nutritional and financial support. Non-governmental organizations provided substantial support, with participants expressing greater satisfaction with NGO assistance compared to governmental programs.

Conclusion: Despite progress in pediatric HIV management, challenges persist in Dakshina Kannada, especially in ensuring equitable access to nutrition and financial support. Collaborative efforts between governmental and non-governmental entities are crucial to address gaps and provide comprehensive care for affected children.

Key Words: Children and Adolescents Living With HIV/AIDS, Opportunistic infections, Antiretroviral therapy (ART), Government initiatives, Non-governmental organizations (NGOs).



PP-CP-013: Variation in labelling of various brands of Paracetamol available in Goa

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The present study aimed to evaluate the primary labelling of various paracetamol brands available across pharmacies in Goa, with a focus on compliance with the Drug and Cosmetics Act, 1940 and Rules, 1945. A total of 55 paracetamol products were collected from multiple sources, including Hindu Pharmacy (Panaji), Apollo Pharmacy, Wellness Pharmacy, and others in Margao and Vasco. The products included 30 tablets, 8 drops, 15 suspensions, 1 suppository, and 1 infusion. Label contents were assessed across 12 parameters, including composition, warning statements, dosage instructions, presence of generic name, inclusion of Hindi/Devanagari, and patient information.

Findings indicated notable variation among labels, particularly in format, dosing instructions, and additional information. While most products complied with general labelling rules, significant inconsistencies were observed—such as absence of overdose warnings on some labels and varying dosage instructions based on age or weight. Few products included therapeutic use or clear directions, potentially leading to consumer confusion. Droppers and measuring cups were sometimes inadequately marked or partially obscured, affecting dosing accuracy.

The study also highlighted a lack of patient information leaflets, especially for non-prescription products, and minimal inclusion of critical safety warnings seen in international labelling standards. Although many products included the generic name prominently and featured Hindi text, further standardization is necessary. Recommendations include introducing a standardized labelling format for over-the-counter medications, including all essential warnings, dosage guidelines, and possibly Braille labelling. A simple, clear, and informative label design should be a priority to enhance patient safety and usability in India.



PP-CP-014: EEG-Based Seizure Prediction in Epilepsy Using Deep Learning: A Clinical Decision-Support Approach

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Background:

Uncontrolled epilepsy presents a significant clinical burden, with unpredictable seizures posing safety risks and impacting quality of life. In pharmacy practice, there is growing interest in predictive technologies that support patient-centered care and therapeutic decision-making. Deep learning (DL) offers potential to analyze electroencephalogram (EEG) data for early seizure prediction, enabling timely interventions and adherence strategies.

Objective:

To develop and evaluate a deep learning-based model that predicts seizure risk using non-invasive scalp EEG recordings, supporting proactive clinical management in epilepsy.

Methods:

EEG data from the CHB-MIT database, comprising long-term scalp recordings of pediatric epilepsy patients, was preprocessed and segmented into 30-second windows. Each segment was labeled as pre-ictal (within 30 minutes before seizure) or interictal (baseline). A hybrid deep learning model combining 1D Convolutional Neural Networks (CNN) with Long Short-Term Memory (LSTM) networks was implemented to capture both spatial and temporal EEG dynamics. Model performance was evaluated using accuracy, sensitivity, specificity, and ROC-AUC.

Results:

The model achieved an overall accuracy of 89.2%, sensitivity of 91.5%, specificity of 87.3%, and ROC-AUC of 0.93. It demonstrated strong ability to identify early seizure signatures from EEG. These results highlight the clinical utility of DL models in real-time seizure risk prediction and patient counseling.

Conclusion:

This study presents a promising AI-based framework for seizure prediction using EEG, with potential integration into clinical pharmacy practice through wearable alerts, medication adherence tools, and pharmacist-led epilepsy care. Personalized prediction models may empower patients and reduce seizure-related morbidity.

Keywords:

Seizure prediction, Epilepsy, EEG, Deep learning, Clinical pharmacy, CNN-LSTM, Patient safety, Neuropharmacy

PP-CP-015: Advancing myocardial infarction risk prediction with troponin and CK-MB: a Shap-based machine learning framework for clinical decision-making.

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Background:

Myocardial infarction (MI) remains a leading cause of cardiovascular mortality worldwide. Accurate and early risk assessment is crucial for improving patient outcomes. This study developed a machine learning (ML)-based predictive model utilizing key cardiac biomarkers, troponin and creatine kinase-MB (CK-MB), to enhance MI diagnosis.

Objective:

To compute a MI risk score using ML algorithms and integrate SHapley Additive exPlanations (SHAP) to improve interpretability and clinical decision-making.

Methodology:

ML classifiers including Random Forest, XGBoost, and Decision Tree were trained on data from 1,319 patients with nine clinical variables. Data preprocessing involved normalization, feature encoding, and hyperparameter tuning. Models were evaluated using accuracy, precision, recall, F1-score, and AUC. SHAP analysis was employed to explain model predictions and assess feature importance.

Results:

Tree-based models achieved over 97% accuracy. SHAP analysis identified age, CK-MB, and troponin as the most impactful predictors, enhancing transparency and clinical relevance.

Conclusion:

ML combined with SHAP explainability offers strong potential for MI prediction, supporting early diagnosis and informed clinical decisions. Future research should incorporate larger datasets and additional variables to boost predictive performance.

Keywords: Myocardial Infarction, Machine Learning, Troponin, CK-MB, SHAP, Predictive Modeling, Explainable AI, Cardiovascular Risk.



PP-CP-016: Impact of patient counselling in the management of medications and pharmaceutical care in geriatric patients in the tertiary care hospital

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Background: Geriatric patients often face polypharmacy, poor adherence, and limited understanding of medications, leading to adverse outcomes. Patient counselling is a fundamental aspect of clinical pharmacy services, particularly in geriatric care, where medication adherence and understanding are crucial for improved health outcomes. Clinical pharmacist-led counselling plays a significant role in educating elderly patients about their medications, lifestyle modifications, and safety measures.

Aims & Objectives: To assess the impact of structured patient counselling on medication adherence, disease awareness, and overall well-being in geriatric patients. The primary objective was to evaluate the effectiveness of clinical pharmacy services in improving adherence, health literacy, and understanding of medications.

Methods: A prospective observational study was conducted over six months in a tertiary care hospital, involving 132 geriatric patients aged 60 years and above. Customized questionnaire forms were provided to assess patient knowledge, medication adherence, and lifestyle habits before and after counselling sessions. Patients received structured counselling on medication use, potential side effects, lifestyle modifications, and safety measures. Pre- and post-counselling assessments were conducted to measure the impact.

Results: Among 132 patients, 63.64% received direct counselling, while 36.36% had their representatives counselled. Post-counselling evaluations showed significant improvements, with disease and medication awareness. Physical activity levels improved, with 49.24% of patients engaging in frequent activity post-counselling compared to 40.91% before. Dietary habits also showed enhancement, with percentage of patients rating their diet as “excellent” rising from 9.09% to 19.7%. Additionally, safety awareness increased from 64.39% pre-counselling to 99.24% post-counselling.

Conclusion: This study highlights the significant impact of clinical pharmacy services on patient counselling in geriatric care. The use of customized questionnaire forms and structured counselling sessions significantly improved medication adherence, disease awareness, and lifestyle modifications. Expanding these services in healthcare settings can further enhance geriatric patient outcomes.

Keywords: Clinical pharmacy services, Patient counselling, Geriatric care, Medication awareness.



PP-CP-017: Randomised placebo-controlled trial of synbiotics in live donor liver transplantation performed for patients with acute on chronic liver failure

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Background:

Patients with Acute-on-Chronic Liver Failure (ACLF) who undergo living donor liver transplantation (LDLT) have a heightened risk of post-transplant mortality, often due to infections originating from the gut. Synbiotics may help to restore gut microbiota in such individuals. This study explores whether synbiotic supplementation can mitigate infectious complications in this high-risk group.

Aims:

To evaluate the efficacy of perioperative synbiotics in reducing infections among ACLF patients undergoing LDLT through a randomised controlled trial.

Methods:

In this double-blind, placebo-controlled study, 44 ACLF patients scheduled for LDLT were randomly assigned to either a synbiotic group (n = 21; VSL#3®: 3 capsules/day and Yogut®: 1 capsule/day) or a placebo group (n = 23). The intervention started 3 days pre-transplant and continued for 6 weeks post-surgery. The primary outcome was infection occurrence within 6 months post-transplant. Secondary outcomes included complications (graded using the Modified Clavien–Dindo system), ICU/hospital stay duration, antibiotic usage, and mortality. Statistical tests included the Wilcoxon rank-sum for continuous data and Fisher's exact for categorical variables.

Results:

Patients receiving synbiotics had a shorter ICU stay than those in the placebo group (median 7 vs 10 days; p = 0.05). Infection rates were slightly lower in the synbiotic arm (33%) than in the placebo arm (39%), though the difference was not statistically significant (p = 0.76). Postoperative INR levels were significantly higher in the placebo group (median 3.0 vs 2.4; p = 0.03). Other outcomes, such as liver function, biliary issues, rejection episodes, and mortality, showed no marked differences between groups.

Conclusion:

Perioperative synbiotic therapy may help reduce ICU stay and postoperative infections in ACLF patients undergoing LDLT, suggesting a potential supportive role in post-transplant care.

Keywords: Gut microbiota, ACLF, Synbiotics, Probiotics, Prebiotics, Living donor liver transplantation

PP-CP-019: "Theranostics in precision oncology: Bridging

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Background:

Independent Ethics Committees (IECs) are central to ensuring the ethical conduct of clinical research in India. They are tasked with safeguarding participant rights, ensuring scientific and ethical protocol adherence, and maintaining documentation standards. However, failures in IEC functioning have led to ethical controversies, notably in the PATH HPV vaccine trial and clinical testing on survivors of the Bhopal gas tragedy. With a surge in clinical trials, particularly industry-sponsored ones, the need for robust and accountable ethics oversight has become critical.

Aims and Objectives:

This study aims to critically examine the operational shortcomings of IECs in India and to identify systemic issues that hinder the proper implementation of prescribed ethical guidelines. The objective is also to propose practical and evidence-informed reforms that can enhance the ethical governance, functionality, and independence of these committees within the country's evolving clinical research landscape.

Methods:

A qualitative desk review was conducted, including the Indian Council of Medical Research (ICMR) Ethical Guidelines (2017), New Drugs and Clinical Trials Rules (NDCTR, 2019), CDSCO registration norms, journal articles, and case reports. Case studies such as the PATH HPV trial, Bhopal Gas Aftermath Tragedy trials, and the Covaxin trial were thematically analyzed to identify patterns in ethical non-compliance. A stakeholder survey may be conducted in the future to strengthen insights.

Results:

The analysis revealed recurring issues: irregular IEC meetings, lack of quorum, inadequate training, poor documentation, delays in SAE review, conflicts of interest, and weak enforcement. These gaps persist despite comprehensive regulatory frameworks.

Conclusion:

To bridge the gap between regulation and reality, India must institutionalize mandatory training, enforce centralized audits, support independent IECs, and adopt tiered review systems. To ensure ethical integrity.

Keywords:

Independent Ethics Committee, Clinical Research, India, Regulatory Gap, ICMR Guidelines, NDCTR, Ethical Oversight

PP-CP-020: Independent Ethics Committees in India: An Assessment of Regulations vs. Reality

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Background:

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This study aims to critically examine the operational shortcomings of iecs in India and to identify systemic issues that hinder the proper implementation of prescribed ethical guidelines. The objective is also to propose practical and evidence-informed reforms that can enhance the ethical governance, functionality, and independence of these committees within the country's evolving clinical research landscape.

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To bridge the gap between regulation and reality, India must institutionalize mandatory training, enforce centralized audits, support independent iecs, and adopt tiered review systems. To ensure ethical integrity.

Keywords:

Independent Ethics Committee, Clinical Research, India, Regulatory Gap, ICMR Guidelines, NDCTR, Ethical Oversight



PP-CP-021: A Meta-Synthesis on the Therapeutic Applications, Resistance Mechanisms, and Safety Profile of Fluconazole.

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Background:

Fluconazole is a widely used antifungal agent known for its effectiveness, oral availability, and safety in treating fungal infections. Fluconazole is used for fungal infections affecting mucosal surfaces (mouth, oesophagus, vagina), bloodstream, urinary tract, lungs, peritoneum, and central nervous system caused primarily by *Candida* and *Cryptococcus* species. However, the increasing incidence of resistance among certain fungal species and emerging safety concerns have brought its long-term clinical utility into question.

Aims & Objectives:

The therapeutic efficacy of fluconazole and mechanisms of emerging resistance are assessed in this meta-synthesis. Safety of fluconazole in different patient groups is also examined. The aim is to look for patterns, gaps, and research directions in the use and stewardship of fluconazole.

Methods:

A systematic review of peer-reviewed literature published in the last two decades was conducted using databases such as PubMed, Scopus, and ScienceDirect. Studies included clinical trials, observational studies, and in vitro analyses focusing on fluconazole's efficacy, resistance mechanisms, and safety outcomes. Clinical implications and themes were identified from the data.

Results:

Fluconazole continues to be active against the majority of fungal infections in immunocompetent patients. Resistance among non-albicans *Candida* and other opportunistic fungi has, however, been increasing. Major resistance mechanisms involve gene mutations in the ERG11 gene, overexpression of efflux pumps, and biofilm-related tolerance. Except for hepatotoxicity, drug interactions, and teratogenicity when administered in pregnancy, fluconazole is otherwise well tolerated.

Conclusion

Although fluconazole remains a useful antifungal drug, the development of resistance and safety issues underscore the importance of rational prescribing, monitoring of resistance, and antifungal stewardship. Ongoing research and clinical alertness are necessary to maintain its continued efficacy and safe use.

Keywords:

Fluconazole, antifungal resistance, safety profile

PP-CP-022: HER2 Positive Breast Cancer as a Secondary Malignancy in Patients receiving Imatinib Mesylate for Chronic Myeloid Leukaemia

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Introduction

Imatinib, (TKI's) a first-generation is used as a first line therapy in treating CML. It acts on BCR-ABL1 gene, and participates in cellular signal transduction as well as in numerous cellular activities such as cell division, and proliferation. Secondary malignancies can occur in the course of CML; however, they are extremely rare.

*TKI's Tyrosine Kinase Inhibitors

Case Report

A 48-year-old female patient presented at our study hospital was diagnosed with CML [BCR-ABL P210 Transcript detected with BCR-ABL score of 3.554%] and was initiated with Tablet Imatinib 400mg Daily. Patient responded well to Imatinib therapy with BCR-ABL at 0.024% in 6 months. During the 8th month of Imatinib therapy, patient presented with a cancerous lump in the left breast, and underwent upfront BCS. Histopathology reported stage I (pt2n0mx) Breast cancer, Immunohistochemistry revealed ER/PR-ve, HER2 +ve and Ki 67- 15%.

Patient was started on 1st cycle TCH regiment with, Inj Docetaxel 110mg + Inj Carboplatin 400mg + Inj Trastuzumab 440mg and Imatinib therapy was continued concurrently, patient completed 1st cycle of TCH without any adverse effects.

Discussion

The annual incidence of CML with breast cancer is 127 instances per 1,00,000 patients. There are very few cases that has previously reported CML and secondary cancers occurring simultaneously. Recent studies also revealed that Imatinib has potential to increase secondary tumours however retrospective evaluations of CML patients taking tkis revealed comparable or even lower rates of secondary cancers compared to the general population.

Conclusion

Although this does not conclusively imply whether patient co-existence of both malignancy is a coincidence, it is suggested to observe such maladies.



PP-CP-023: A Prospective Observational Study on Health-Related Quality of Life Among Elderly Cancer Patients

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Background:

Cancer in the elderly poses unique clinical and psychosocial challenges, often impacting their overall health-related quality of life (HRQoL). As aging is associated with comorbidities and functional decline, cancer diagnosis and treatment may further compromise physical, emotional, and social well-being. Understanding HRQoL in this population is essential for developing patient-centered care strategies that address not only disease outcomes but also life satisfaction, independence, and mental health.

Aims and Objectives

- To determine the HRQOL among the study patients.
- To determine the domains affected among aged cancer patients.

Methodology

A prospective observational study was conducted for 3 months where cancer patients of any gender ≥ 60 years were enrolled. All necessary data like patient demographics were obtained from various data sources including medical records, treatment charts etc. The HRQOL of study patients was assessed using the Centre of Disease Control Health-Related Quality of Life -14 Scale (CDC-HRQOL-14) by one through one interview with the patient.

Results

A total of 50 patients were enrolled into the study. 92% of the patients rated their general health either as very good (12%), good (40%) or fair (40%). Many of these patients reported that physical health (52%) and mental health (56%) were not good ≥ 10 days. Based on the activity limitation module, 84% of the patient's activities were limited because of a health problem, most commonly cancer (88%). A larger (80%) group of study patients needed the help of others in handling their routine needs. According to the healthy days module, 72% of patients were in pain and did not get sufficient sleep (56%) for at least 10 days.

Conclusion

Even though most of the study subjects perceived their general health positively, physical, and mental health were impaired along with limitations in their activity almost regularly



PP-CP-024: Triamcinolone acetonide in refractory prurigo nodularis: a rare case report

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Background:

Prurigo nodularis (PN) is an unusual chronic inflammatory skin disorder characterized by strongly pruritic, hyperkeratotic, and well-defined nodules on the extensor surfaces of the limbs and trunk. However the exact etiology was unknown, and it is often thought to be idiopathic. Atopic dermatitis, chronic kidney failure, diabetes, hyperthyroidism, iron deficiency anemia and hepatitis B and C, HIV are among the systemic, dermatological and infectious that have been connected to it. Histopathological examination of PN reveals hyperkeratosis, acanthosis, dermal fibrosis, and a mixed inflammatory infiltrate. Managing prurigo nodularis is difficult, with patients often undergoing many therapy regimens that yield unsatisfactory outcomes.

Aims & Objectives:

- To describe a case of long-standing prurigo nodularis in a 58-year-old male
- To evaluate the clinical course and treatment resistance in this patient.

Methods:

A 58-year-old male patient with a 10-year history of prurigo nodularis was evaluated. He had previously tried topical and systemic anti-inflammatory medications and antihistamines, with no significant relief. A skin biopsy was performed for diagnostic confirmation.

Results:

The patient presented with multiple well-defined, hyperpigmented, firm-to-hard nodules over the extensor and lateral aspects of both lower limbs, some with central oozing and crusting. The ankles and dorsum of the foot were covered in hyperpigmented plaques with lichenification. Fundoscopy showed that the left eye's lens and right eye's visual activity (6/12). Contributing factors identified included poorly controlled diabetes and nutritional deficiencies. The patient was managed with intralesional Triamcinolone acetonide and supportive topical and systemic therapies.

Conclusion:

Therefore, Triamcinolone acetonide is an inhibitor of Glucocorticoid is a promising choice for the treatment of PN and with no adverse effects. In which cytokines are the main inflammatory factors causing pruritic. In the future, greater sample numbers and multi-ethnic clinical trials will be required to give stronger evidence.

Keywords:

Triamcinolone acetonide: Biopsy: pruritis: skin nodules: Diabetes mellitus.



PP-CP-025: A Study on the Prevalence of Childhood Obesity Among School Children in Kalaburagi

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Background:

Childhood obesity has emerged as a significant public health concern in India, with WHO reporting an 18% prevalence rate. Rapid urbanization, sedentary lifestyles, and unhealthy dietary habits contribute to this growing issue. Obesity in childhood often leads to health complications in adulthood.

Aims & Objectives:

To assess the prevalence of obesity among school children in Kalaburagi city and identify key contributing factors

Methods:

A 6-month prospective, observational school-based study was conducted across various schools in Kalaburagi. Students were enrolled based on defined criteria, and assent was obtained. Data was collected using a structured form before and after an educational intervention. Body Mass Index (BMI) was calculated using height and weight to determine obesity levels. Educational leaflets were distributed, and post-intervention data was analyzed to assess impact and awareness.

Results:

BMI Classification: Underweight: 30.49%, Healthy weight: 47.19%, Overweight: 16.88%, Obese: 5.44%

Gender Trends: 52.81% of overweight/obese children were male.

Age-wise Prevalence: Highest in 14-year-olds (42.67%), Lowest in 16-year-olds (13.79%)

Class-wise Distribution: 9th Grade: 48.2%, 10th Grade: 16.5%

Risk Factors: Genetics: 14.93%, Lack of physical activity: 17.32%, Unhealthy diet: 17.86%

All combined: 49.89%

Conclusion:

Obesity prevention should begin early through school-based initiatives, active sports participation, regular health check-ups, and parental awareness. Collaborative efforts involving teachers, parents, and students are essential to control the rising trend of childhood obesity.

Keywords:

Overweight, Obesity, Nutrition, WHO



PP-CP-026: Relapse of pemphigus vulgaris following rituximab: a case report highlighting the role of alcohol use and poor glycaemic control

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Background:

Pemphigus vulgaris (PV) is an autoimmune blistering disorder characterized by intraepithelial acantholysis due to autoantibodies against desmogleins. Rituximab, a CD20-directed monoclonal antibody, is increasingly recognized as a first-line treatment for moderate-to-severe PV. Despite its efficacy, relapses may occur, especially in the presence of modifiable risk factors.

Aims & Objectives:

To present a case of PV relapse following rituximab therapy and highlight the role of metabolic and lifestyle factors—specifically chronic alcohol use and poor glycaemic control—in influencing disease recurrence and management outcomes.

Methods:

We present the case of a 60-year-old man with a known diagnosis of PV who experienced a relapse following multiple cycles of rituximab (administered according to the rheumatoid arthritis protocol). Clinical examination, laboratory investigations, and treatment interventions were documented.

Results:

The patient presented with widespread mucocutaneous erosions and vesiculobullous lesions, with positive Marginal Nikolsky and Asboe-Hansen signs. Contributing factors identified included poorly controlled diabetes, nutritional deficiencies, and recent resumption of chronic alcohol consumption. Laboratory results showed leukocytosis, hypoalbuminemia, microcytic hypochromic anemia, and slightly abnormal liver function tests. The patient was managed with high-dose corticosteroids, azathioprine, and supportive topical and systemic therapies.

Conclusion:

While no direct causal relationship has been established between alcohol use and PV relapse, this case underscores the potential impact of lifestyle factors and metabolic instability on treatment outcomes. To our knowledge, there are limited case reports describing alcohol-induced PV relapse. This case emphasizes the significance of lifestyle changes and thorough patient education are to the long-term treatment of autoimmune skin conditions.

Keywords:

Pemphigus vulgaris, Rituximab, Alcohol use, Immunosuppressive therapy, Glycemic control



PP-CP-027 : Shaping the future of pharmacy & healthcare innovation through pharmex card & application

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Background:

The global healthcare landscape is rapidly evolving with the integration of digital technologies aimed at improving patient outcomes, reducing errors, and enhancing the efficiency of care delivery. Traditional pharmacy practice often relies on paper-based prescriptions and fragmented communication between patients, pharmacists, and healthcare providers, leading to increased risks of medication errors, poor adherence, and disrupted continuity of care. With the growing demand for personalized and accessible healthcare, there is a pressing need for innovative systems that can digitize and streamline pharmaceutical services. Smart card technology and mobile health applications have emerged as promising tools to bridge these gaps, enabling the centralization of patient health data, improved tracking of medication usage, and real-time coordination among healthcare stakeholders. The PHARMEX Card & Application was conceptualized as a forward-thinking solution to these challenges. By integrating pharmacy records, patient information, and communication capabilities into a secure and user-friendly digital platform, PHARMEX aims to revolutionize how pharmaceutical care is delivered. This initiative supports national goals of digital health transformation and seeks to create a patient-centric, technologically empowered ecosystem that fosters proactive health management and informed decision-making.

Aims and Objectives:

1. To digitize pharmaceutical services using a smart card and mobile application.
2. To enhance communication between patients, pharmacists, and healthcare providers.
3. To improve prescription tracking, inventory management, and patient adherence.

Methods:

1. Developed PHARMEX as an integrated platform for patient data, prescriptions, and pharmacy transactions.
2. Included features: digital refills, reminders, e-consultations, and centralized health records.
3. Implemented with user-friendly design and secure data management.

Results:

1. Improved prescription adherence and reduced medication errors.
2. Enhanced pharmacist workflow and inventory control.
3. Better patient engagement and continuity of care across facilities.

Conclusion:

PHARMEX bridges digital innovation with pharmacy practice, enabling smarter, patient-centered healthcare. It supports national digital health goals and transforms service delivery at both individual and system levels.

Keywords:

Digital Health, Pharmacy Innovation, Smart Card, Patient Care, PHARMEX, Healthcare Technology

PP-CP-028: Zuranolone-only oral drug for Postpartum Depression (PPD)

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Like other major depressive disorders, Postpartum Depression (PPD) can be life-threatening, which occurs during pregnancy or within 4 weeks of postpartum involving symptoms like anxiety, physical changes, depression, anhedonia and can be as dangerous as self-harm. The primitive cause of PPD is a dramatic drop in the neuroprotective hormones like estrogen and progesterone, post delivery. It can also occur due to domestic violence, unintended pregnancy, familial history of psychotic disorders and absence of social support. Its an overlooked but globally prevalent disorder found in every 1 out of 8 women, and in India, 22% of pregnant women experience it.

PPD is induced via deficiency of estrogen which in turn increases the uptake of serotonin, affecting the GABA release. Decreased amount of progesterone and its cerebral metabolite(allopregnanolone) result in increased irritability and stress.

Zuranolone, being the first and only oral drug treating PPD, is an synthetic analogue of allopregnanolone and works by allosterically modulating GABA receptor and tailoring the release of GABA synaptically and extra-synaptically.

This FDA-approved drug has been subjected to clinical trials(double-blind, placebo-controlled trial) where both groups were subjected to 14days of the respective drugs. The group that received Zuranolone showed better symptoms than the group that received placebo.

Hence, this drug must be given once daily (30mg or as prescribed) for 14 days ,and overdosing must not be tolerated as the drug clearance is poor.

Side effects include somnolence, diarrhea, fatigue and a low chances of UTI infection. The patient must not drive or do any vigorous activity within the first 12 hours of administering the medicine.

Therefore, this drug stands out due to its advantages over the existing IV infusions.



PP-CP-029: Resmetirom: Pioneering the fight against Non-Alcoholic Steato Hepatitis (NASH) with First- Ever FDA Approval

Supreetha Nayak

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Non-Alcoholic Steatohepatitis (NASH) is a progressive liver disease characterized by steatosis, lobular inflammation, ballooning degeneration, and fibrosis, unrelated to alcohol consumption. Its prevalence is increasing worldwide due to rising obesity, diabetes, hypertension, and insulin resistance, with genetics also playing a significant role.

Approximately 15-25% of NASH patients develop cirrhosis, which can lead to hepatic carcinoma, subacute death, or NASH recurrence, contributing to 30-40% of liver-related deaths. Symptoms include fatigue, abdominal pain, and hepatomegaly. Conventional treatment focuses on lifestyle modifications, weight loss, and managing comorbidities, alongside antioxidants, Vitamin E, and Pioglitazone.

In March 2024, Resmetirom (marketed as Rezdiffra) became the first FDA-approved drug for NASH. This life-saving medication prevents hepatic cirrhosis and reverses fibrosis when combined with lifestyle modifications. Resmetirom is a selective thyroid hormone receptor beta agonist that enhances fatty acid β -oxidation, reduces intrahepatic triglycerides and inflammation, suppresses hepatic sterol regulatory element-binding protein, and improves liver function. It has 84% of the activity of T3 on THR-beta receptors.

Rezdiffra is Administered orally at 80 mg (<100 kg) or 100 mg (>100 kg) once daily, with or without food, Resmetirom is metabolized by the CYP2C8 enzyme, requiring dose adjustments when used with inhibitors like Gemfibrozil. The MAESTRO-NASH 52-week trial showed 29.9% NASH resolution in patients receiving 100 mg, compared to 14.2% in the placebo group. The drug was well tolerated in clinical trials, with nausea and vomiting reported in >10% of patients. Warnings include potential gallbladder-related side effects and liver toxicity. However, Resmetirom has shown limited benefits in decompensated steatohepatitis patients.

Conclusion: Being the first and the orally approved drug, Resmetirom keeps a crucial step forward in NASH management, addressing an urgent medical need and improving patient outcomes.



PP-CP-030: AI-Driven Cardiovascular Care: From Early Diagnosis to Personalized Therapeutics

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Background:

Cardiovascular diseases (cvds), a group of heart and blood vessel disorders, remain one of the most prevalent diseases claiming 17.9 million lives each year. Conventional methods, though effective, often fail to manage the complexity of cvds, which causes delay in personalised treatment decisions especially for high-risk therapies like anticoagulation, when relied on trial-based approaches. The integration of Artificial Intelligence can improve early diagnosis, risk grouping and personalized treatment, bridging the therapeutic – diagnostic gap in clinical practice.

Aims & Objectives:

Focused on machine learning (ML) models supporting cardiovascular care covering two critical domains: (1) routine clinical variables used for early disease detection, and (2) individualized warfarin dosing and International Normalized Ratio (INR) control. It aims to explore AI's role in connecting data-driven pharmaceutical research with optimized patient therapy.

Methods:

Multiple peer reviewed studies were analyzed. Global research trends were identified through bibliometric mapping. ML models, namely Random Forest (RF), Decision Tree (DT), K Nearest Neighbor (KNN) were assessed for the detection of CVD using hospital data. Furthermore, ML was used to predict warfarin maintenance doses and stabilize INR in patients on anticoagulation.

Results:

The bibliometric analysis revealed expanding use of AI in cvds and therapeutic decision making. ML based diagnostic models demonstrated >89% accuracy using non-invasive inputs. Dosing models used for warfarin improved prediction accuracy and INR control, along with minimizing adverse events throughout the treatment cycle.

Conclusion:

AI helps in reducing clinical uncertainty and improves personalized care in cardiovascular treatment. This dual application illustrates a data driven bridge between pharmaceutical research and measurable therapeutic outcomes.

Keywords:

Artificial Intelligence, Cardiovascular Disease, Machine learning, Warfarin, INR, Risk Prediction, Personalized Therapy.



PP-CP-031: AI-Driven Clinical Decision Support: Redefining the Role of the Clinical Pharmacist

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Background:

Artificial Intelligence (AI) is increasingly being integrated into healthcare to improve the speed and accuracy of clinical decision-making. In pharmacy, AI-powered Clinical Decision Support Systems (CDSS) are emerging as valuable tools that support pharmacists in ensuring safer and more effective medication use.

Aim and Objectives:

This review aims to highlight how AI-driven CDSS enhances the role of clinical pharmacists. The objectives are to understand how these systems support medication review, therapy optimization, and patient safety, while strengthening interdisciplinary collaboration.

Methods:

A narrative review was conducted using published literature, case studies, and healthcare models involving AI in pharmacy practice. These sources were analyzed to evaluate the benefits, applications, and challenges of AI-CDSS.

Results:

AI-CDSS tools have shown the ability to identify drug interactions, flag high-risk prescriptions, and assist in accurate dosing. These systems help reduce medication errors, streamline pharmacist workflows, and improve communication with physicians.

Conclusion:

AI-driven CDSS enhances, rather than replaces, the clinical pharmacist's role by supporting evidence-based, personalized care. Successful adoption requires proper training, ethical use, and data security measures.

Keywords:

Artificial Intelligence, Clinical Pharmacy, CDSS, Pharmacist Role, Medication Safety, Healthcare Technology



PP-CP-032: Cost-Effectiveness Analysis of Biosimilar Vs Innovator Biologics in Rheumatoid Arthritis Treatment in India

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Background:

Biologic therapies have revolutionized rheumatoid arthritis (RA) management but remain prohibitively expensive for many patients in India. The introduction of biosimilars offers a potential pathway to improve affordability and access, yet concerns regarding their comparative value and acceptance linger.

Objective:

To evaluate the cost-effectiveness and patient uptake of biosimilar biologics compared to originator (innovator) biologics for RA treatment in the Indian healthcare setting.

Method:

A mixed-methods approach was used, including analysis of published pricing data, Prescription patterns, and patient surveys in tertiary care centres. Direct medical costs, drug accessibility, and clinical outcomes were assessed for both biosimilars and innovator products.

Results:

Biosimilar biologics were priced 30–50% lower than their innovator counterparts, reducing out-of-pocket costs for patients and enabling greater initiation of biologic therapies. Comparable rates of clinical remission and adverse effects were observed between biosimilars and originators. However, hesitancy among both prescribers and patients owing to perceived efficacy and safety concerns affected the biosimilars market.

Conclusion:

Biosimilar adoption leads to substantial cost savings without compromising clinical effectiveness, thus expanding therapeutic options for RA patients in India. Persistent misconceptions and regulatory uncertainties need to be addressed through targeted education and robust post-marketing surveillance to bolster confidence in biosimilars. Broader acceptance of this alternative among healthcare providers and patients is essential for realizing their full potential, promising both economic and clinical benefits.

Keywords:

Biosimilar, rheumatoid arthritis, cost-effectiveness, India, Biologics, drug affordability, healthcare utilization



PP-CP-033: Bacteria and the Brain: A Probiotic Love Story Exploring Cognition and the Gut-Brain Axis

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Background:

The gut-brain axis (GBA) is a bidirectional communication system linking the gut microbiota with the central nervous system, influencing emotional and cognitive processes. Psychobiotics, a subset of probiotics, are emerging as novel modulators of mental health and cognitive function through their impact on the microbiome-gut-brain signaling pathways.

Objective: This review explores the role of probiotics in modulating brain function, emotional regulation, and cognition by analyzing preclinical and clinical evidence, mechanistic pathways, and potential therapeutic applications.

Methods:

We synthesized findings from high-quality studies published between 2020 and 2024, focusing on mechanisms such as neurotransmitter modulation, immune regulation, gut permeability, hypothalamic-pituitary-adrenal (HPA) axis modulation, and glycemic control. Emerging tools including AI-driven microbiome profiling and multi-omics integration were also examined.

Results:

Probiotic strains such as *Lactobacillus rhamnosus* GG, *Bifidobacterium longum*, and *Lactobacillus helveticus* exhibit promising effects on anxiety, depression, stress, and cognitive function through modulation of GABAergic signaling, serotonin synthesis, and inflammatory cytokines. Probiotics also enhance glycemic control, suggesting a link between metabolic health and cognitive resilience. Clinical trials support their efficacy, though variability in strains, dosing, and study designs presents limitations.

Conclusion:

Psychobiotics represent a promising, non-pharmacological strategy for enhancing mental health and cognition. However, standardization, mechanistic clarity, and longitudinal trials are needed. The integration of personalized probiotic therapy through precision nutrition and AI technologies may redefine mental healthcare and lifestyle medicine.

Keywords:

Gut-brain axis, probiotics, psychobiotics, cognition, mental health, neurotransmitters, HPA axis, glycemic index, personalized nutrition, microbiota.



PP-CP-034: Impact of Patient Care Interventions on Clinical, Humanistic, and Treatment Outcomes of Tuberculosis Patients with Diabetes Mellitus: A Systematic Review

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Background: Tuberculosis (TB) and diabetes mellitus (DM) are major global health concerns that frequently coexist, particularly in low- and middle-income countries. This dual burden negatively affects disease progression and outcomes. Patient care interventions have shown promise in improving outcomes in chronic conditions, but their role in TB patients with DM (TB-DM) co-management remains unclear.

Aims & Objectives:

To systematically review the impact of patient care interventions on clinical, humanistic, and treatment outcomes among TB-DM patients.

Methods:

A comprehensive literature search was conducted in pubmed, Embase, and Scopus from inception to April 2025 and was registered in PROSPERO (International Prospective Register of Systematic Reviews) with registration number: CRD420251024621. Interventional studies evaluating the effects of patient care interventions in adults with TB-DM comorbidity were included. Outcomes were categorized as clinical (e.g., glycemic control), humanistic (e.g., patient knowledge, adherence), and treatment-related (e.g., TB treatment success). The risk of bias was assessed using the Cochrane ROB tool. A narrative synthesis was performed due to heterogeneity in interventions and outcomes.

Results:

Three rcts conducted in Malaysia and Indonesia between 2021 and 2023 met the inclusion criteria. Interventions included structured patient educational counselling, glucose monitoring, and medication adherence support. Two studies observed improved glycemic control, while all reported enhanced patient knowledge and adherence. Only one study reported TB treatment outcomes, showing improved cure and success rates post-intervention. The overall risk of bias was low to moderate.

Conclusion:

The evidence suggests that patient care interventions may improve clinical and humanistic outcomes, and potentially treatment outcomes, in TB-DM patients. These findings support integrating structured patient support strategies into multidisciplinary care models for TB-DM comorbidity. Further large-scale, multicenter trials are needed to validate these findings and assess the long-term impact.

Keywords:

Tuberculosis, Diabetes Mellitus, Patient Care Intervention, Glycemic Control, Treatment Adherence, Systematic Review



PP-CP-035: Artificial Intelligence-Based Adherence Prediction for Non-Communicable Diseases

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Background: Medication non-adherence is a critical challenge in the management of chronic non-communicable diseases (NCDs), contributing significantly to suboptimal therapeutic outcomes, increased hospitalizations, and elevated healthcare costs. Artificial Intelligence (AI) and Machine Learning (ML) offer innovative approaches to predict and monitor adherence behaviors, thereby enabling timely and personalized clinical interventions.

Aim and Objectives

To use AI to predict medication adherence and improve outcomes in non-communicable diseases.

Objectives include

- Identify key factors affecting medication adherence.
- Develop AI/ML models for adherence prediction.
- Evaluate models using accuracy, sensitivity, specificity, and AUC.
- Apply models to diseases like diabetes, CVD, and asthma.
- Enable early intervention through prediction.

Methods: This study leverages AI models trained on heterogeneous data sources, including electronic dosing records, audio logs, smart pill dispensers, refill histories, and data from wearable sensors. Deep learning architectures, particularly Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTM) networks, were employed to analyze temporal and multimodal data for adherence prediction. Model performance was assessed using metrics such as accuracy, sensitivity, specificity, F1 score, and area under the receiver operating characteristic curve (AUC-ROC).

Results: Experimental results indicate that AI-based systems can predict non-adherence with high accuracy (>77%) and robust AUC values (~0.84). Disease-specific models demonstrated effective prediction in conditions such as Type 2 diabetes, cardiovascular diseases (e.g., lipid-lowering therapy), schizophrenia, inflammatory bowel disease, Parkinson's disease, and asthma. Real-time monitoring using ingestible sensors and video-based systems further enhanced prediction reliability.

Conclusion: AI-enabled adherence prediction represents a transformative tool for proactive healthcare delivery. By facilitating early identification of at-risk patients, these systems support targeted, individualized interventions, potentially reducing clinical deterioration and optimizing resource allocation. Future implementation requires rigorous external validation, attention to algorithmic fairness, and seamless integration into clinical decision-support systems.

Keywords

Artificial Intelligence (AI), Machine Learning (ML), Long Short-Term Memory, Non-adherence

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Date: 28th – 30th August 2025

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