



Drug Design and Drug Discovery Discussion Group of IPA Kerala State branch

# National Conference on Drug Design and Discovery



Date: 24th & 25th October, 2025

Jointly Organized by
IPA
Kerala State Branch

Department of Pharmaceutical Chemistry
Amrita School of Pharmacy

#### **Patrons**

#### Dr. Shantikumar V Nair

Associate Provost of Academics Amrita Vishwa Vidyapeetham

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#### Dr. P Jayasekhar

President

IPA Kerala State Branch

#### Dr. Sabitha M

Principal

Amrita School of Pharmacu

# Co-Chairperson

#### Dr. John Joseph

Hon. Secretaru

IPA Kerala State Branch

# **Advisory Committee from DDDS Discussion Group**

#### Dr. K. Krishna Kumar,

Principal,

St. James College of Pharmaceutical Sciences, Chalakudy

#### Dr. David Paul

Assistant Professor,

Department of Pharmaceutical Analysis,

NIPER, Kolkata

#### Dr. Aravind A

Associate Professor of Medicinal Chemistry, Govt. College of Pharmaceutical Sciences, Thiruvananthapuram

#### Dr. Sapna Shrikumar

Principal

Ahalia School of Pharmacy

Palakkad

#### Dr. Sutharson L

Principal,

Nirmala College of Health Science,

Chalakudy

#### Dr. Biju CR

Vice Principal & Professor, Devaki Amma Memorial College of Pharmacy,

Malappuram

#### Dr. Arun Rasheed

Vice Principal & Professor, Al Shifa College of Pharmacy,

Malappuaram

#### Dr. Bijo Mathew,

Professor & HOD of Pharmaceutical Chemistry, Amrita School of Pharmacy, Kochi.

#### Dr. Preeja G Pillai

Principal,

Mar Dioscorus College of Pharmacy,

Thiruvananthapuram

#### Dr. Aneesh TP

Associate Professor & HOD. Dept. of Pharmaceutical Chemistry, Amrita School of Pharmacy, Kochi

#### Dr. Akash Marathakam

Professor & HOD, Dept. of Pharmaceutical Chemistry, Sree Gokulam College of Pharmacy, Alappuzha

#### Dr. Badmanaban

Principal.

Nirmala College of Pharmacy

Muvattupuzha

# **Local Organizing Committee:**

Dept. of Pharmaceutical Chemistry, Amrita school of Pharmacy

Chairperson: Dr. Aneesh T P, HOD

#### **Members**

Dr. Bijo Mathew

**Professor** 

Dr. Leena K Pappachen

**Associate Professor** 

Dr. Subin Mary Zachariah

**Associate Professor** 

Dr. Saiprabha V N

Assistant Professor

# **Pre-Conference Workshop**

Maximum No. of Participants: 40

As a curtain-raiser to the National Conference, a hands-on Preconference Workshop has been designed to empower participants with practical skills in computational drug discovery techniques. The workshop focuses on two high-impact modules:

#### **Module 1: Molecular Docking Studies**

Led by Dr Bijo Mathew, Professor,

Dept of Pharmaceutical Chemistry, Amrita school of Pharmacy

**Software Used: MZ Dock** 

**Session Aides: Ms Sachithra S** 

(PhD Scholars Amrita school of Pharmacy)

This module introduces participants to the fundamentals of molecular docking, a key in silico tool in structure-based drug design. Using MZ Dock, participants will gain insights into:

- · Basics of ligand-receptor interactions
- Protein and ligand preparation
- Docking protocol setup and execution
- Scoring functions and interpretation of binding results
- · Case studies demonstrating application in hit identification

This session is ideal for beginners and intermediates aiming to explore virtual screening and binding affinity predictions in early-stage drug discovery.

#### Module 2: Network Pharmacology

Led by Dr. Aneesh T P, Associate Professor & HOD,

Dept. of Pharmaceutical Chemistry, Amrita school of Pharmacy

Software Used: STRING Database & Cytoscape

Session Aides: Ms Sonu Benny, Mr. Vishnu V R (PhD Scholars Amrita school of Pharmacy)

This module provides an overview of systems-level drug discovery using network pharmacology approaches, enabling participants to:

- Identify and construct protein-protein interaction (PPI) networks
- Use the STRING database for target prediction and functional enrichment analysis
- Visualize and analyze biological networks using Cytoscape
- · Interpret network topology and identify key regulatory nodes
- Apply network pharmacology to multi-target drug design and disease pathway mapping

Participants will walk away with a strong foundation in integrating biological data for multi-target drug discovery and mechanism-of-action prediction.

The National Conference on Drug Design and Discovery is a premier academic event aimed at exploring the next frontiers in pharmaceutical innovation. As the drug discovery landscape undergoes a technological revolution, this conference brings together leading researchers, industry professionals, academicians, and students to discuss transformative trends and technologies shaping the future of drug development. The conference will focus on integrating artificial intelligence (AI), machine learning (ML), target-based screening, molecular dynamics, and computational tools to accelerate the identification, optimization, and validation of novel therapeutic agents. With increasing demand for precision medicines and faster R&D pipelines, the event provides a timely platform to examine how digital technologies are driving the shift from traditional drug discovery methods to more efficient, data-driven approaches.

#### **Conference Objectives:**

- · To highlight recent advances in Al and ML applications in drug design
- · To showcase the role of target-based screening and molecular modeling
- · To encourage young researchers to engage in computational drug discovery
- To provide hands-on experience through preconference workshops on molecular docking and network pharmacology

#### **Academic and Professional Enrichment**

Participants will benefit from expert lectures, interactive sessions, case studies, and poster presentations, covering both foundational knowledge and emerging trends. Eminent speakers from academia and industry will share their insights, research findings, and success stories in the following areas:

- Artificial Intelligence in Drug Design
- Molecular Dynamics Simulations
- Structure- and Ligand-Based Virtual Screening
- Network Pharmacology and Systems Biology

#### Why Attend?

- Stay updated with cutting-edge technologies in drug design
- Network with domain experts and fellow researchers
- · Gain practical exposure to computational tools through hands-on workshops
- Present your research and receive feedback from experts
- · Discover opportunities for collaboration and interdisciplinary learning

We welcome students, scholars, faculty members, and professionals from pharmacy, life sciences, biotechnology, chemistry, and data sciences to join this enriching experience.



**Dr. T. K. Manoj Kumar,**Professor & Dean (Research),
School of Digital Sciences,
Digital University Kerala

Topic: Al and GenAl Applications in Anti-Cancer Drug Design



**Dr. Dhivya Shanmugarajan**Manager – Scientific Specialist,
Dept of Life Sciences, BIOVIA
ALTEM.

Topic: Significance of AI in Drug Design and Development



**Dr. Bijo Mathew,**Professor, Department of
Pharmaceutical Chemistry,
Amrita School of Pharmacy.

Topic: Molecular Dynamics: A look inside the invisible world of molecules.



Dr. Wilbee DS
CM's Nava Kerala Post
Doctoral Fellow &
Assistant Professor in
Pharmaceutical Chemistry
Govt. Medical Cillege
Thiruvananthapuram
Topic: Precision targeting:
Advancing Drug Discovery
through Computer Aided
Target Based Screening

#### **Call for abstracts for Poster Presentation**

We are pleased to invite students, researchers, faculty members, and industry professionals to submit abstracts for poster presentations at the upcoming National Conference on Drug Design and Discovery.

Poster presentations serve as a dynamic platform for showcasing original research, case studies, and innovative methodologies in the field of drug discovery.

Scientific papers may be submitted under (but not limited to) the following categories:

- 1. Al in Drug Discovery
- 2. Pharmaceutical & Analytical Chemistry
- 3. Pharmaceutics & Drug Delivery
- 4. Pharmacology & Toxicology
- 5. Phytochemistry & Pharmacognosy
- 6. Pharmacy Practice & Clinical Research

**Certificates of participation** will be awarded to all presenters.

**Best Poster Awards** will be presented to the outstanding entries, with recognition to the presenting authors.

Note: Submissions are not limited to the categories listed above. Authors are welcome to present work on allied topics relevant to the conference theme

#### **Poster Presentation Guidelines**

#### 1. Content & Structure

A scientific poster should follow a logical flow that includes the following sections:

- Title: Clear, informative, and concise. Should reflect the essence of the study.
- Authors & Affiliations: Include full names, designations, and institutional affiliations.
- Introduction/Background: Brief overview and rationale for the study.
- Objectives: Clearly stated aim(s) of the study.
- · Methodology: Concise description of methods used (materials, study design etc.).
- Results: Key findings presented through figures, tables, and bullet points.
- Discussion: Interpretation of results, limitations, and relevance.
- · Conclusion: summary of findings.
- References (if applicable): Only the most relevant and recent references (limit to 3-5).
- Acknowledgments: Optional, to thank contributor's/funding agencies.

# **Poster Design**

#### Size & Dimensions:

Standard size is usually 36" x 48" (3 ft x 4 ft) in landscape or portrait format.

#### Layout:

- · Use columns for better readability.
- Keep spacing between sections for clarity.

#### **Font Sizes:**

- Title: 72–100 pt,
- Headings: 36-48 pt,
- Body text: 24–32 pt,
- Captions/References: 18–24 pt

#### **Color Scheme:**

- Use high-contrast colors.
- Prefer a light background with dark text.
- Avoid overly bright or clashing color schemes.

#### Visuals:

- Use graphs and diagrams instead of heavy text.
- Ensure images are of high resolution (300 dpi or above).
- Label all figures and tables properly.

#### Sustainable and Eco-friendly Practices

- Use recycled or biodegradable materials for printing posters wherever possible.
- Avoid plastic lamination; consider reusable fabric-based posters.

A well-prepared poster presentation reflects both the quality of your research and your ability to communicate it. Use this opportunity not only to share your findings but also to connect, collaborate, and grow as a researcher.

Best wishes for a successful presentation!

Sent your abstract to (email id)

#### **Important Dates:**

Early Bird registration: 30<sup>th</sup> September 2025

Last date for abstract submission: 10th October 2025

Notification of Acceptance: 12<sup>th</sup> October 2025 Last date for Registration: 14<sup>th</sup> October 2025

Workshop & Conference Dates: 24<sup>th</sup> & 25<sup>th</sup> October 2025

# **Registration Fees**

Category	Workshop Only	Conference Only	Both Workshop & Conference	Early Bird
UG/PG Students	₹ 1000	₹ 750	₹ 1500	₹ 1300
IPASF members	₹ 900	₹ 650	₹ 1300	₹ 1100
IPA Members	₹ 1400	₹ 900	₹ 2000	₹ 1800
Research Scholars/ Faculty /Industry	₹ 1500	₹ 1000	₹ 2200	₹ 2000

### For Registration Scan this QR Code



#### **Contact & Queries:**

pharmaprincipal@aims.amrita.edu

Mob: 9447556410,

9400939292, 9388019388



# ACCOMMODATION AVAILABLE NEAR THE VENUE

## **HOTELS**

MATHA RESIDENCY NON A/C SINGLE - INR 1008 NON A/C DOUBLE- INR 1500 A/C SINGLE - INR 1500 A/C DOUBLE - INR 1750 (P) 0484 2800429

COCHIN RESIDENCY TWO BED A/C- INR 1300 TWO BED NON A/C- INR 800 (P) 94761 93506

KIRA PALACE RESIDENCY A/C DOUBLE- INR 2200 A/C DELUXE- INR 2800 (P) 77363 72757 BLUEMOON (VGR)
NON A/C- INR 100QTWO BED)
A/C- INR 1500(TWO BED)
A/C - INR 1800(THREE BED)
Discounted Rat@Inclusive Tax): 5%

OMNEST A/C SINGLE- INR 1650 A/C DOUBLE- INR 2250 (P) 0484 2802023

(P) 87147 53357

GHALA RESIDENCY NON A/C- INR 1500 A/C DOUBLE- INR 2200 (P) 80897 10727

- \* Delegates are requested to contact the hotel directly for booking your preferred stay prior to the event
- \* Rates are excluding of food charges.