RAMAIAH UNIVERSITY OF APPLIED SCIENCES

Faculty of Pharmacy

# DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

IN ASSOCIATION WITH

Zastra Innovations
solutions to innovate...

Organizes Two Days

# 5th International Workshop

ON

## "COMPUTATIONAL TOOLS IN DRUG DESIGN"

## CTD2-2025

## 28th and 29th November 2025

### KEY TOPICS OF WORKSHOP

- Hit Identification
- Virtual Screening
- Homology Modelling
- LBDD
- Library Enumeration
- Protein-Protein Docking
- ADMET
- MD Simulations, FEP
- ML-QSAR

- Solubility Solvent/Solute Screening
- API Co-Crystal Screening
- Excipient Screening Stoichiometry
- Optimization
- Membrane Studies & Formulations
- Hansen Parameters
- QSPR

## Target Audience

*Faculties , PhD Scholars, PG Students*

- Pharmacy
- Chemistry
- Biotechnology
- Life & Allied Sciences

LIMITED SEATS

1 + 1 MONTH COMPLIMENTARY SOFTWARE ACCESS

BIOVIA | CompuTherm FOR MATERIALS DESIGN | alvascience

**Registration Fee: 1500/- (Incl GST)**

**Registration Link**

cresset CADD software | ACD/Labs | CDD VAULT Complexity Simplified

***Last date for Registration : 20-11-2025***

**For Queries:** *fph_pharmachem@msruas.ac.in* | *+91 - 9629396767*

RAMAIAH UNIVERSITY OF APPLIED SCIENCES

# Faculty of Pharmacy

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Head
Dept. of Pharmaceutical Chemistry, FPH, RUAS

## Organizing Secretary

**Dr. Parasuraman P**
Associate Professor
Dept. of Pharmaceutical Chemistry, FPH, RUAS

## About the Workshop

Computational Tools in Drug Design – CTD2-2025 delivers an end-to-end, hands-on pipeline that balances discovery and developability. Participants will map targets using Network Pharmacology, perform Hit Identification and Virtual Screening, build structures using Homology and Pharmacophore Modelling, and evaluate interactions using Protein–Protein and Ligand Docking. You'll expand SAR with Library Enumeration, guide series by LBDD, boost predictivity using ML-QSAR and Ligand EC Alignment Design, and confirm binding/stability with Molecular Dynamics (MD) and FEP. In parallel, the pre-formulation track covers QSPR-based solubility, Hansen Parameters, Solvent/Solute selection, API Co-Crystal and Excipient screening, Stoichiometry optimization, and Membrane Studies & Formulations. This workshop delivers a comprehensive, end-to-end understanding of drug design–from *in-silico* discovery (Docking, MD, ML-QSAR) to preformulation and developability.

## Ramaiah University of Applied Sciences

Ramaiah University of Applied Sciences (RUAS) is a state private university, under the aegis of Gokula Education Foundation. The innovative university focuses on academics, research, consultancy, training and leadership development. RUAS offers outcome-based education in health and allied sciences, engineering, and humanities. RUAS is oriented towards student-centric education and services with applied research whilst maintaining the highest academic and ethical standards in a creative and innovative environment. RUAS inspires critical thinking, personal development, and a passion for lifelong learning. RUAS is accredited with A+ Grade by NAAC.

## Faculty of Pharmacy

Faculty of Pharmacy (FPH), formerly M.S. Ramaiah College of Pharmacy, was established in 1992. Faculty of Pharmacy, ranked 56 in the AIR– NIRF 2025, is a leading Pharmacy college with a legacy of 33 years. It imparts outcome-based pharmaceutical education to meet the growing demands of well-trained healthcare professionals globally. The faculty offers B.Pharm (NBA-Accredited), Pharm.D, M.Pharm in Pharmaceutical Chemistry, Pharmaceutics, Pharmacology, Pharmacognosy, Pharmacy Practice, Regulatory Affairs, and Ph.D programme.

## Department of Pharmaceutical Chemistry

Department of Pharmaceutical Chemistry was originally established as a part of M S Ramaiah College of Pharmacy. PG program in Pharmaceutical Chemistry was started in the year 2008. The department was integrated into Faculty of Pharmacy in 2014. The department provides outcome-based education and training skills on various aspects of drug design using bioinformatics and computational tools, synthesis by conventional and green chemistry approaches, spectral characterization, and pharmacological evaluation of small molecules. Moreover, students get practical training in handling various advanced instruments including Microwave synthesizer, ATR-IR, Flame photometer, HPLC, HPTLC and utlising GPU powered Computational Lab.

## Zastra Innovations

Zastra Innovations is a leading provider of scientific software and services, with a proven track record of success in helping our customers achieve their goals. Zastra was founded in 2015 by a team of scientists with a deep understanding of the challenges and opportunities facing the Indian scientific community. Zastra is at the forefront of innovation in the field of machine learning and AI, and is working with its partners to develop new solutions in the areas of drug discovery and materials science. The company is committed to helping Indian researchers achieve their goals and advance scientific discovery.

For Queries: fph_pharmachem@msruas.ac.in ; +91 - 9629396767