

Faculty of Pharmacy







Department of Pharmaceutical Chemistry **Organizes Two Days**

3rd International Workshop

on

"Computational Tools in Drug Design - CTDD"

22nd and 23rd September 2022

HIGHLIGHTS

SIFT, PredictSNP, STRING, Cytoscape, PyRx, Autodock Vina, Pymol, Discovery Studio, PkCSM, Pharmagist, ZINCPharmer, BuildQSAR, DESMOND







₹ Registration Fee: Rs. 1500/- (Inclusive of Taxes)

Limited Participants Only





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Dr. Harish Kumar D R
Professor and Head
Department of Pharmaceutical Chemistry
FPH, RUAS



Organizing Co-ordinator

Dr. Parasuraman. P
Assistant Professor
Department of Pharmaceutical Chemistry
FPH, RUAS



About the Workshop

Drug design and drug discovery is a passionate, prolonged, and inter-disciplinary multistep process. The traditional drug discovery process is costly and time-consuming which demands hard work. The in silico approach has become indispensable for the drug discovery process. The in silico methods have been proved beneficial in the estimation of biological activities of chemical compounds against a target. Moreover, it has been used to examine the binding affinities towards the target and also used in the prediction of physicochemical properties depending upon their molecular and structural features of a broad range of chemical compounds. Besides, computational screening seems an important method to limit the cost, time, and manpower in comparison to the traditional drug discovery process. This hands-on workshop summarizes the importance and applications of various aspects of in silico approaches along with the case studies where in silico methods have been applied in the drug discovery process.

About Ramaiah University of Applied Sciences

Ramaiah University of Applied Sciences (RUAS) is a private university established by an Act of the State of Karnataka, India, sponsored by the Gokula Education Foundation. Ramaiah University is an innovation university that focuses on academics, research, consultancy, training and leadership development. The university offers outcome-based multidisciplinary education in the domains of medical, paramedical, engineering, life sciences and social sciences. RUAS is oriented towards student-centric professional 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. This university has been rated as a "FIVE STAR" Institution by the Karnataka State University Rating Framework (KSURF) - 2019 Government of Karnataka.

About Faculty of Pharmacy

The Faculty of Pharmacy (FPH), formerly M.S. Ramaiah College of Pharmacy, was established in 1992. The Faculty of Pharmacy, ranked 62nd in the AIR– NIRF 2022, is a leading Pharmacy college with 30 years of legacy. It imparts outcome based pharmaceutical education to meet our country's growing demands of well-trained healthcare professionals. The faculty offers a 4-year undergraduate programme - Bachelor of Pharmacy degree (B. Pharm), 2-year Postgraduate programme - Master of Pharmacy degree (M. Pharm) in Pharmaceutics, Pharmacology, Pharmaceutical Chemistry, Pharmacognosy, and Pharmacy Practice, 6-year Doctor of Pharmacy degree (Pharm D), and Doctoral research programme (Ph.D.).

About the 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 conventional and green chemistry approaches, spectral characterization, and pharmacological evaluation of small molecules. Moreover, students get practical training in handling analytical instruments including spectrophotometer, FT-IR, Flame photometer and HPLC.

COURSE CONTENT AND SPEAKERS



Inheritance of ApoE4, early onset in Alzheimer's disease, and discovery of small molecules to impede ApoE4-DNA interactions – A case study



Dr. Meenakshisundaram Balasubramaniam

Assistant Professor and Inglewood Scholar

Department of Geriatrics, University of Arkansas for Medical Sciences,

United States

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SNP Analysis in Drug Design

Dr. Krishna Murthy T P
Assistant Professor

Department of Biotechnology Ramaiah Institute of Technology, Bengaluru, Karnataka, India





Target fishing: An Omics Perspective

Mrs. Gouri Nair

Assistant Professor

Department of Pharmacology

Faculty of Pharmacy, RUAS, Bengaluru, Karnataka, India



Molecular Docking and Molecular Dynamics Simulation in Drug Design

Dr. Parasuraman P

Assistant Professor

Department of Pharmaceutical Chemistry
Faculty of Pharmacy, RUAS, Bengaluru, Karnataka, India





Applications of QSAR in Drug Design

Dr. A. R. Mahesh

Assistant Professor

Department of Pharmaceutical Chemistry
Faculty of Pharmacy, RUAS, Bengaluru, Karnataka, India



Pharmacophore Modelling in Drug Design

Dr. Manikanta Murahari

Associate Professor

K L College of Pharmacy

KL Deemed to be University (KLU), Vijayawada, Andhra Pradesh, India



Computational Tools in Drug Design-CTDD 2022