



Faculty Development Program



VIT[®]
Vellore Institute of Technology
(Deemed to be University under section 3 of UGC Act, 1956)

Title : One Day FDP on Molecular Dynamics, Simulation for Modern Drug Discovery & A Hands-on Training Using BIOVIA Discovery Studio

Date : 2025-12-03 - 2025-12-03

Time : 10:00 - 17:30

Venue : TLCE

Event Outcome

- Understand molecular interactions. Set up



Resource Person 1 - Details

Name : Dr GAURAV KUMAR

Designation : ASSOCIATE PROFESSOR AND HEAD, DEPT OF BIOTECHNOLOGY AND BIOENGINEERING SCHOOL OF BIOSCIENCES AND TECHNOLOGY

University/ Company : GALGOTIAS UNIVERSITY, GREATER NOIDA

Address : INDIA, 203201.



Resource Person 2 - Details

Name : Dr DHIVYA S

Designation : SENIOR APPLICATION SCIENTIST, NATIONAL SUPPORT FOR BIOVIA SOLUTIONS

University/ Company : ALTEM TECHNOLOGIES, CHENNAI

Address : INDIA, 600017.

Resource Person's Profile :

1. Profile of Dr GAURAV KUMAR

Dr. Gaurav Kumar is an associate professor and head of the Department of Biotechnology and Bioengineering and Head of the Institute's Innovation Council at Galgotias University, Greater Noida. He earned his PhD in Biomedical Engineering from IIT BHU Varanasi. With 40 publications, 14 patents, 3 books, and 8 chapters, he has led several funded projects. His research focuses on neuroprotection, wound healing, and drug discovery.

2. Profile of Dr DHIVYA S

Dr. Dhivya is a senior application scientist for BIOVIA Solutions at Altem Technologies, specializing in computational drug discovery, molecular modeling, and simulation. With 45 publications and six book chapters, she blends expertise in protein modeling, RNA Seq, toxicity profiling, and AI-based drug design. As a gold medalist PhD graduate, she has delivered 45 invited talks and trained participants in the 2020 Drug Discovery Hackathon.

Neurodegenerative diseases like Alzheimers, Parkinsons, and Huntingtons are marked by protein misfolding, aggregation, oxidative stress, and inflammation in the brain, leading to loss of neurons. Phytochemicals such as curcumin, resveratrol, quercetin, and catechins display strong antioxidant, antiinflammatory, and neuroprotective effects, but the detailed molecular mechanisms behind these actions are still being investigated. This session reveals how molecular dynamics simulations help researchers visualize and study the dynamic interactions between phytochemicals and important disease proteins in environments that reflect real physiological conditions, including the presence of water, ions, biologically relevant temperatures, and pH levels. Through such simulations, key insights are gained into binding affinity, stability, essential amino acid interactions, conformational changes, and how these compounds can inhibit or stabilize disease-associated proteins. This knowledge is vital for designing new drugs and developing more effective neuroprotective agents. The module targets faculty and researchers in fields like biotechnology, pharmacy, and life sciences, especially those involved in drug discovery, herbal product development, and structural biology. It begins by covering the basics of molecular dynamics such as the use of force fields, potential energy calculations, motion equations, solvation processes, periodic boundary conditions, and various simulation environments. Key workflow steps like protein and ligand preparation, energy minimization, system equilibration, and simulation production are detailed, along with how they affect the accuracy of results. The session also introduces participants to BIOVIA Discovery Studio, highlighting protocol setup, parameter selection, trajectory analysis, and essential visualization tools.

BIOVIA Discovery Studio

Coordinator's: Prof. KRISHNA RAO ESWAR N 20206 - Associate Professor Grade 1 - CNBT
Prof. BALAVIGNESWARAN CK 22410 - Associate Professor Grade 2 - CNBT