

ONLINE WORKSHOP ON

QSAR MODELING

IN

COMPUTER AIDED DRUG DESIGN (CADD)

*Predicting Biological Activity
Through Computational Intelligence*



22-27
JUNE 2026



8:00 PM IST



Live online

ABOUT THE COURSE

This course provides a practical introduction to QSAR modeling and its role in Computer-Aided Drug Design (CADD). Participants will learn how molecular structures are correlated with biological activity to predict drug behavior, and accelerate the drug discovery process.

WHO CAN JOIN?

- UG & PG Students
- Research Scholars
- Faculty Members
- Bioinformatics Scientist
- Pharmaceutical Scientists
- Drug Discovery & Industry Professionals

COURSE OBJECTIVES

- Understand the basics of CADD
- Learn molecular modeling concepts
- Explore QSAR principles and workflows
- Build predictive QSAR models
- Apply statistical validation techniques
- Discover QSAR applications in drug development

RESOURCE PERSON

Dr. Md Afroz Alam

Former Assistant Professor
Department of Bioinformatics Karunya
Institute of Technology and Sciences,
Coimbatore



Get Certificate



Live & Interactive Sessions



Learning Resources & Recordings



Hands-on Training



Doubt Resolution Support



Industry-Relevant Skills

WORKSHOP MODULE

DAY 1 CADD AND MOLECULAR MODELING	<ul style="list-style-type: none">• Introduction to Computer-Aided Drug Design• Molecular Simulation• Force Fields• Energy Minimization
DAY 2 DRUG DEVELOPMENT PROCESS	<ul style="list-style-type: none">• Overview of Drug Discovery Pipeline• Process of CADD• Technology Impact on Drug Development• Methodologies and Strategies
DAY 3 QSAR AND DRUG DESIGN	<ul style="list-style-type: none">• Introduction to QSAR• Steps in QSAR Modeling• Importance of QSAR in Drug Discovery
DAY 4 QSAR DATA ANALYSIS	<ul style="list-style-type: none">• Potential Drug Properties• Molecular Descriptors• Pharmacophore Modeling
DAY 5 MINITAB FOR QSAR	<ul style="list-style-type: none">• Introduction to Minitab• Multiple Linear Regression Models• PRESS Statistics• SSY Analysis
DAY 6 APPLICATIONS OF QSAR	<ul style="list-style-type: none">• Correlation Coefficient Analysis• Model Validation Techniques• Pharmaceutical Applications of QSAR

WHY JOIN THIS WORKSHOP?

- Industry-Relevant Skills
- Hands-On Understanding of QSAR
- Drug Discovery Applications
- Expert-Led Sessions
- Networking with Researchers and Professionals

LEARNING OUTCOMES

- Understand QSAR fundamentals and applications
- Develop QSAR prediction models
- Validate models using statistical methods
- Predict compound biological activity (IC_{50}/pIC_{50})
- Support lead optimization and drug design
- Apply computational tools in drug discovery

REGISTRATION FEE

Indian Participants: ₹999 Only
International Participants: \$ 45 US

