

University of Calicut



in association with



Anusandhan
National
Research
Foundation

Zastra
Innovations



ANRF-PAIR sponsored Workshop on Computer-Aided Drug Design (CADD) Techniques

This training-oriented online workshop series highlights how biological structures power modern drug discovery, taking participants from target identification to lead optimization through expert insights, interactive sessions, and real-world research case studies.

What is covered and objectives?

- Introduction to CADD, molecular modelling studies
- Molecular Docking, Electrostatic Complementarity (EC), Molecular Dynamics
- Case Studies and on-project examples with live demonstrations.

Why to attend?

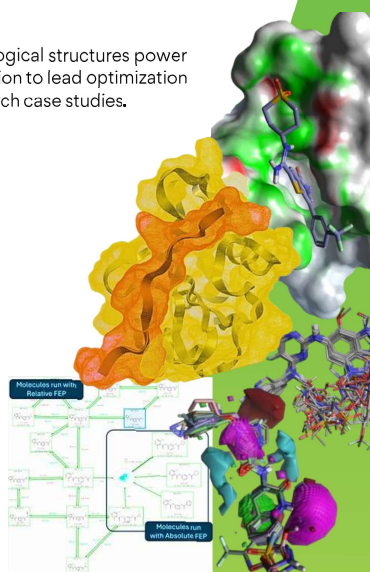
- Gain practical experience in drug discovery software of used in molecular modeling.
- Understand best practices in decision-making from ligand screening and ligand binding analysis.
- Gain insights into in silico approaches to accelerate hit identification and lead optimization.
- Explore pragmatic interpretations from computational predictions.

For Hands-on Workshops:

- Windows/Mac OSX/Linux Laptop
- 4GB RAM, Core i5/Ryzen 5 series CPUs with 5GB HDD storage or higher.
- Tutorials and example files will be shared.
- Training license with software links will be shared to registered attendees.

Who can attend?

- Faculty members from University/Institutes/Colleges
- Scientists, Post-Docs and Research Scholars
- Master Students
- Computational Drug Discovery and Delivery enthusiasts



Mar 11, 2026



10:00 AM to 05:00 PM



University of Calicut



Contact us: Dr. Susmita De (Coordinator) Phone: 94962 13788 Email: susmita@uoc.ac.in



Resource Person



Gopukrishnan R

Senior Scientist (Applications)
Zastra Innovations Pvt Ltd



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Collaborative Science & Research



Our Softwares



Benefits for attending

- 1-Month Free Demo License for hands-on practice
- Advanced Training in CADD Techniques with practical insights
- Comprehensive Workshop Series covering all essential topics
- AI-driven drug discovery in our workshop series.
- Hands-on training with Cresset's Flare, an industry-standard commercial software

Organised by

Department of Chemistry, University of Calicut

Funded by

ANRF-PAIR Project

Zastra Innovations

Phone No : 07907332818

Email: ask@zasttrain.com

Website: www.zasttrain.com



Registration link/Scan QR code :

<https://forms.gle/zHQtyjWhYnNev5Ik6>



Registration fee for external participants : Rs.500/-
Last date for registration : **9th March-2026**

REGISTRATION

9:30 AM - 10:00 AM

Registration

10:00 AM - 11:15 AM

Introduction to Flare features

11:15 AM - 11:30 AM

Tea Break

11:30 AM - 1:00 PM

Hands-On session on Molecular Docking, Electrostatic Complementarity (EC), See and Learn - Ensemble Docking and MMGBSA

1:00 PM - 2:00 PM

Lunch Break

2:00 PM - 3:00 PM

How to setup MD in flare and MD result interpretation

3:00 PM - 3:15 AM

Tea Break

3:15 PM - 4:30 PM

See & Learn for QSAR model building and results analysis

4:30 PM - 5:00 PM

Questions & Answers session

Contact us: Dr. Susmita De (Coordinator) Phone: 94962 13788 Email: susmita@uoc.ac.in