



Workshop Kit and Certificate will be provided

Hands on training on Databases, tools and softwares like Pymol, SwissPDBviewer, Pubchem, Autodock vina, Ligplus, VMD, ADMET, SAVES, MolInspiration will be provided. Work in a Linux platform

THIS WORKSHOP PROVIDES HANDS-ON-TRAINING ON THE MAJOR CONCEPTS IN DRUG DESIGNING THAT INCLUDE

- ✓ Target selection and screening
- ✓ Ligand designing and Optimization
- ✓ In silico methods in ADMET and Toxicity
- ✓ Virtual Screening of ligand libraries
- ✓ Drug-protein Interaction chemistry

Registration Fee
 Student - Rs. 1000/-
 Scholar - Rs. 1500/-
 Faculty - Rs. 2000/-
 Industry - Rs. 3000/-



Scan the QR code or Click the link to register
<https://forms.gle/5xXqRmg6xdLnyduk6>



Marudhar Kesari Jain

College for Women (Autonomous), Vaniyambadi

RECOGNISED UNDER SEC 2(F) & 12(B) OF UGC ACT, 1956 || ACCREDITED WITH "A+"
 GRADE BY NAAC (4TH CYCLE) PERMANENTLY AFFILIATED TO THIRUVALLUVAR
 UNIVERSITY || AN ISO 21001:2018 (EDMS) CERTIFIED INSTITUTION || MARUDHAR NAGAR,
 CHINNAKALLUPALI, VANIYAMBADI - 635 751.
 WEBSITE: [HTTP://WWW.MKJC.IN](http://www.mkjc.in)



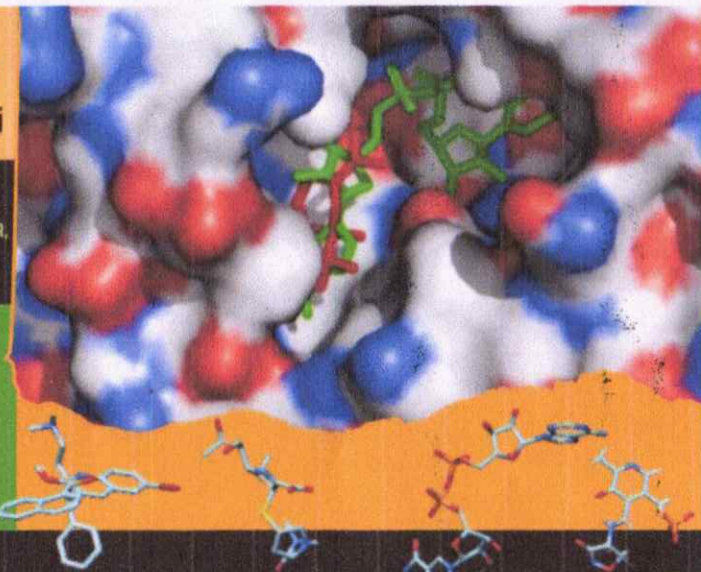
FIST Supported 2 Weeks Workshop on Computer Aided Drug Designing

From 17-11-2025 to 29-11-2025

Computer Aided Drug Design (CADD) has become an indispensable tool in shaping the paradigm of therapeutics. The advent of modern equipment and softwares have made it possible to achieve targeted therapies that are more precise and efficient. CADD has been the backbone for the discovery of several notable drugs such as Dorzolamide, Boceprevir, Captopril, Zanamivir to name a few. Several pharmaceutical and Biotechnological companies rely on CADD for designing and synthesising novel drugs with improved efficacy. CADD also supports in reducing the cost, time and to overcome any real time challenges faced during every stage of the drug development process.

For further details contact :
 Dr. R. Jesu Jaya Sudan
 Associate Dean-Research

Marudhar Kesari Jain College for Women, Vaniyambadi
 Ph. No. +91 9894170894; Email ID: jesu.r@mkjc.in



Outcome of the Workshop

- Understand the concepts of Drug designing
- Become familiar with softwares and Tools in Drug Designing
- Acquire knowledge on protein chemistry
- Obtain practical skills to model and optimise ligands
- Learn molecular aspects of Drug-Protein Interactions
- Visually observe the different methods of target inhibition
- Theoretically evaluate drug likeness and its efficacy

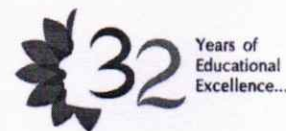
Last date for registration: 10-11-2025
PRINCIPAL

Marudhar Kesari Jain College
 Student, Scholar and Faculty from the disciplines of
 Botany, Biochemistry, Biophysics, Chemistry, Computer Science, English, Health Science, Hindi, Kannada, Malayalam, Marathi, Mathematics, Physics, Sanskrit, Tamil, Telugu, Urdu, and Yoga are eligible
 Vaniyambadi - 635 751
 Tirupattur District



**MARUDHAR KESARI JAIN COLLEGE FOR WOMEN
(AUTONOMOUS) VANIYAMBADI**

Recognised u/s 2(f) & 12(B) by UGC Act, 1956 ||
Permanently Affiliated to Thiruvalluvar University ||
Accredited by NAAC with "A+" Grade ||
An ISO 21001:2018 Certified Institution || Supported by DST-FIST



**DST - FIST SUPPORTED WORKSHOP ON COMPUTER AIDED DRUG
DESIGNING**

Date: 17-11-2025 to 29-11-2025

Agenda

Day	Date	Topic	Theory Sessions	Practical Sessions
1	17-11-2025	Introduction to CADD	Overview of Computer aided drug design	-
2	17-11-2025	Bioinformatics for CADD	Databases for CADD	Databases- Pubmed, Uniprot, OMIM, PDB
3	18-11-2025	Types of CADD	Structure based drug design- Introduction	Literature study- Pubmed
4	18-11-2025	Drug Targets	Target Selection and Screening	Selection of Drug targets- Uniprot , PDB
5	19-11-2025	Active site/Pocket Identification	Visualization of Protein structure	Uniprot, Pymol
6	20-11-2025	Homology Modeling	Concepts and Sequence search tool-BLAST	Selection of Template- Blast
7	20-11-2025	Homology Modeling	Validation of target structure	SwissPDBviewer, SAVES
8	21-11-2025	Ligand	Preparation of ligands	Drug bank, Pubchem
9	22-11-2025	Molecular Docking	Docking with Autodock and analysis	Autodock, Ligplot
10	24-11-2025	Types of CADD	SBDD, LBDD	Docking
11	25-11-2025	Pharmacophore & QSAR	Concepts	Zinc-Pharmer, Molinspiration
12	26-11-2025	Ligand Screening	Virtual Screening	Ligand databases
13	27-11-2025	ADMET	Pharmacokinetics & Pharmacodynamics	PreADMET
14	28-11-2025	Protein Motion	Conformational changes	VMD
16	29-11-2025	Valediction	Presentation by participants, Feedback and Distribution of Certificates	

<https://mkjc.in/research/>


RESEARCH & DEVELOPMENT
PRINCIPAL
Marudhar Kesari Jain College
for Women (Autonomous)
Vaniyambadi - 635 751.
Tirupattur District

3



**MARUDHAR KESARI JAIN
COLLEGE FOR WOMEN (AUTONOMOUS), VANIAMBADI**



Activity Report

Name of the Department / Club / Cell	Research and Development Cell		
Title of the Programme / Event	DST-FIST Supported Two weeks Workshop on Computer Aided Drug Designing		
Alignment of this Programme with	SDGs <input type="checkbox"/> Viksit Bharat 2047 <input type="checkbox"/> State / National Schemes <input type="checkbox"/> NEP 2020 <input type="checkbox"/> MOU activity <input type="checkbox"/> Others <input checked="" type="checkbox"/>		
Mode	Physical mode		
Type of Activity	Workshop		
Level	Institutional level		
Date	17/11/2025 - 29/11/2025	Time	09:30am-12:45pm
Venue	DST-FIST LAB		
Resource Person Details	Dr. J. Lesitha Jeeva Kumari Research Associate cum Assistant Professor PG & Research Department of Biotechnology		
Objective of the programme	To provide a hands-on-training and impart theoretical knowledge on the various bioinformatics concepts related to drug design, tools and software for the participants		
Internal Participants count	Students: 3 Faculty: 7	External Participants count	Students: Nil Faculty: Nil

Report:

DST-FIST supported two weeks workshop on Computer Aided Drug Designing was organised by Research and Development Cell from 17/11/2025 till 29/11/2025. Around ten participants registered for the workshop. Both the theory and the practical sessions were handled by Dr. J. Lesitha Jeeva Kumari. The workshop offered comprehensive hands-on training covering the fundamental concepts of drug design. Key areas included target identification and selection, ligand optimization, pharmacokinetics, pharmacodynamics, virtual screening, drug-likeness evaluation, and drug-drug interactions. Participants were introduced to several widely used databases and computational tools, including Drug Bank, Uniprot, Protein Data Bank, PubChem, PyMOL, SwissPDB Viewer, AutoDock Vina, SAVES etc.

Participants were trained to visualize protein structures, domains, and binding sites using various molecular visualization tools such as PyMOL and SwissPDB Viewer. These sessions enhanced their understanding of protein–ligand interactions and structural biology concepts relevant to rational drug design. The program enabled participants to develop a clear understanding of drug design workflows while gaining practical experience with essential computational tools and software. Practical sessions were provided at the end of every session to reinforce learning outcomes. On the valedictory day, participants shared their feedback and the program concluded with the distribution of certificates.

Outcome of the Program:

- The participants gained a deeper insights into the concepts of computer aided drug desinging.
- The participants gained a practical knowledge in working with the bioinformatics tools and softwares as applicable to computer aided drug designing.
- The participants also gained knowledge on the industrial applications of the concepts and the relative softwares.


Feedback Link : <https://forms.gle/gs8dq34N4925unda7>

Feedback Summary:


The Computer Aided Drug Designing workshop received a positive feedback from the participants. The participants stated that all the concepts were effectively delivered by the resource person. The parrticipants also mentioned that the workshop was very informative, well structured, and highly beneficial for their academics and research. The participants have also suggested to have such advanced level workshops in future.



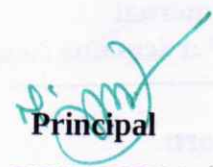
Workshop Mentor



Associate Dean- Research
Dr. R. JESU JAYA SUDAN
Associate Dean - Research
Marudhar Kesari Jain College for Women
Vaniyambadi - 635 751.



IQAC Director



Principal
PRINCIPAL
Marudhar Kesari Jain College
for Women (Autonomous)
Vaniyambadi - 635 751.
Tirupattur District

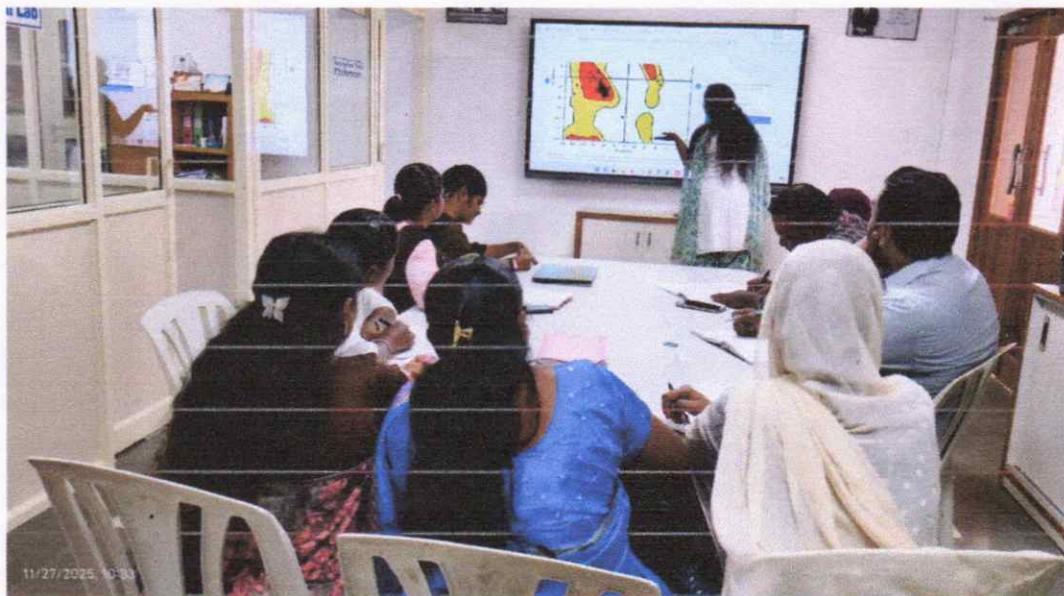
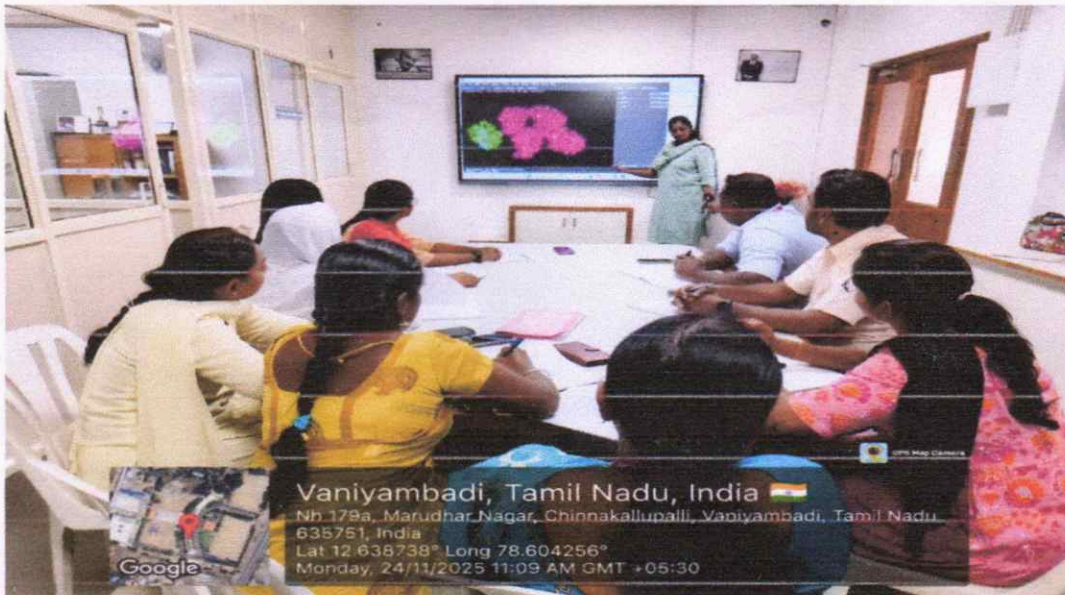


**Marudhar Kesari Jain
College for Women (Autonomous), Vaniyambadi
Research and Development Cell (RDC)**

Programme Name: Workshop

**Topic: "DST-FIST Supported Two weeks Workshop on Computer Aided
Drug Designing"**

Date: 17.11.2025 to 29.11.2025



Ms. [Signature]

PRINCIPAL
Marudhar Kesari Jain College
for Women (Autonomous)
Vaniyambadi - 635 751.
Tirupattur District