

Marudhar Kesari Jain College for Women, Autonomous



Recognized 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 (EOMS) Certified Institution ||
Marudhar Nagar, Chinnakallupalli, Vaniyambadi - 635
751. Website: www.mkjc.in



Scan the QR code or click the
link to register
[https://forms.gle/
AkunynS1jC3NhMhv7](https://forms.gle/AkunynS1jC3NhMhv7)



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.

2 Weeks DST- FIST Supported Internship on

COMPUTER AIDED DRUG DESIGNING

Internship Highlights

This workshop provides hands-on-training on the major concepts in drug designing that include

- Target selection and screening
- Ligand Optimization
- Pharmacokinetics
- Pharmacodynamics
- Drug likeness
- Virtual Screening
- Drug Interactions

Outcome of the Workshop

Understand the concepts of Drug designing
Become familiar with softwares and Tools in Drug Designing
Gain insights into selecting ideal drug targets
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
Gain the ability to work in Linux platform

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

Students, Scholars and Faculty from all disciplines of Life Sciences are eligible

Limited seats
only.
Batch will be
filled on first-
come basis

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

Registration Dates
Batch I - 18th Apr to 30th Apr
Batch II - 25th Apr to 9th May
Batch III - 9th May to 22nd May
Internship & Project- 27th Apr to 30th May

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

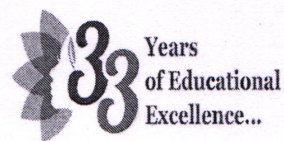
For further details contact :

Dr. R. Jesu Jaya Sudan

Associate Dean-Research, DST-FIST Lab Incharge
Marudhar Kesari Jain College for Women, Vaniyambadi
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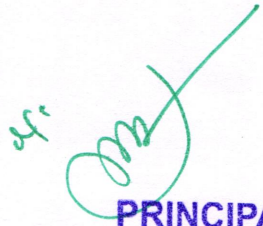


DST-FIST Supported two weeks Internship on Computer Aided Drug Designing

Date: 05-05-2026 to 16-05-2026

Agenda

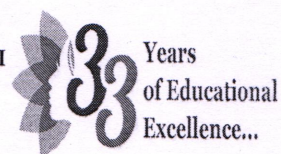
Day	Date	Topic	Theory Sessions	Practical Sessions
1	05-05-2026	Introduction to CADD	Overview of Computer aided drug design	-
2	05-05-2026	Bioinformatics for CADD	Databases for CADD	Databases- Pubmed, Uniprot, OMIM, PDB
3	06-05-2026	Types of CADD	Structure based drug design- Introduction	Literature study- Pubmed
4	07-05-2026	Drug Targets	Target Selection and Screening	Selection of Drug targets- Uniprot , PDB
5	07-05-2026	Active site/Pocket Identification	Visualization of Protein structure	Uniprot, Pymol
6	08-05-2026	Homology Modeling	Concepts and Sequence search tool-BLAST	Selection of Template- Blast
7	08-05-2026	Homology Modeling	Validation of target structure	Swiss PDB viewer, SAVES
8	09-05-2026	Ligand	Preparation of ligands	Drug bank, Pub chem
9	11-05-2026	Molecular Docking	Docking with Autodock and analysis	Autodock, Ligplot
10	12-05-2026	Types of CADD	SBDD, LBDD	Docking
11	13-05-2026	Pharmacophore & QSAR	Concepts	Zinc-Pharmer, Molinspiration
12	14-05-2026	Ligand Screening	Virtual Screening	Ligand databases
13	15-05-2026	ADMET	Pharmacokinetics & Pharmacodynamics	PreADMET
14	15-05-2026	Protein Motion	Conformational changes	VMD
16	16-05-2026	Valediction	Presentation by participants, Feedback and Distribution of Certificates	


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Activity Report

Name of the Department / Club / Cell	Research and Development Cell		
Title of the Programme / Event	DST-FIST Supported Two weeks Internship on Computer Aided Drug Designing		
Alignment of this Programme with	SDGs ☐ Viksit Bharat 2047 ☐ State / National Schemes ☐ NEP 2020 ☐ MOU activity ☐ Others ☒		
Mode	Physical mode		
Type of Activity	Internship		
Level	Institutional level		
Date	05-05-2026 to 16-05-2026	Time	09:30am-1.30pm
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: 15 Faculty: Nil	External Participants count	Students: Nil Faculty: Nil

Report:

The DST-FIST supported two-week Internship on Computer Aided Drug Designing (CADD) was organized by the Research and Development Cell from 05-05-2026 to 16-05-2026. Around fifteen participants registered for the internship. Both theoretical and practical sessions were conducted by Dr. J. Lesitha Jeeva Kumari, providing participants with comprehensive hands-on training in the fundamental principles of drug design. The internship covered key areas including target identification and selection, ligand optimization, pharmacokinetics, pharmacodynamics, virtual screening, drug-likeness evaluation, and drug-drug interactions.





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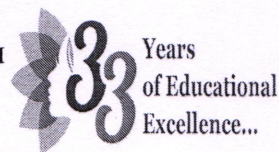
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Participants were introduced to several widely used databases and computational tools such as PyMOL, Swiss-PdbViewer, AutoDock Vina, and PubChem. The training emphasized the visualization of protein structures, domains, and binding sites through molecular visualization software, enabling participants to strengthen their understanding of protein-ligand interactions and essential structural biology concepts relevant to rational drug design. To reinforce conceptual learning, practical sessions were conducted at the end of each module, allowing participants to gain hands-on experience with computational techniques and software applications. Overall, the internship provided participants with a clear understanding of the drug design workflow while enhancing their practical skills in computer-aided drug discovery tools. The program concluded with a valedictory session during which participants shared their feedback, followed by the distribution of certificates

Outcome of the Program:

- The participants gained practical exposure to computational tools and databases used in modern drug discovery.
- The participants Improved hands-on experience in using software such as PyMOL, Swiss-PdbViewer, and AutoDock Vina.
- Increased awareness of the applications of computational biology and bioinformatics in pharmaceutical research.

Feedback Link : <https://forms.gle/grNmW8HQqPpwJLsB9>

Feedback Summary:

The DST-FIST supported Two-Week Internship on Computer Aided Drug Designing (CADD) received an excellent response from the participants. The feedback indicated that the internship was well organized and successfully met its learning objectives. Participants appreciated the clear and effective delivery of both theoretical concepts and practical sessions, which enhanced their understanding of molecular docking, target identification, ligand optimization, and computer-aided drug discovery. Most participants found the programme highly informative, interactive, and beneficial for their academic and research interests. They also expressed satisfaction with the hands-on training and practical exposure provided during the internship. As a suggestion for future programmes, participants recommended including more advanced case studies, extended practical sessions, and providing study materials or recorded lectures for continued learning.

Associate Dean- Research

IQAC Director

Principal

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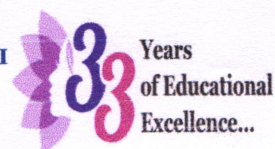
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Research and Development Cell (RDC)

Programme Name: Internship

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

Date: 05-05-2026- 16-05-2026



Principal

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