

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

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.

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PRINCIPAL

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

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

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



Scan the QR code or click the link to register
<https://forms.gle/AkunynS1jC3NhMhv7>



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

For further details contact :

Dr. R. Jesu Jaya Sudan

Associate Dean-Research, DST-FIST Lab Incharge
Marudhar Kesari Jain College for Women, Vaniyambadi
Ph. No. +91 9894170894; Email ID:drjesu2016@gmail.com

Internship 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



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

Date: 18-05-2026 to 30-05-2026

Agenda

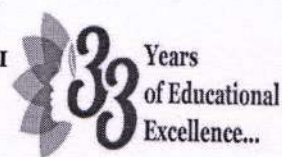
Day	Date	Topic	Theory Sessions	Practical Sessions
1	18-05-2026	Introduction to CADD	Overview of Computer aided drug design	-
2	19-05-2026	Bioinformatics for CADD	Databases for CADD	Databases- Pubmed, Uniprot, OMIM, PDB
3	20-05-2026	Types of CADD	Structure based drug design- Introduction	Literature study- Pubmed
4	20-05-2026	Drug Targets	Target Selection and Screening	Selection of Drug targets- Uniprot, PDB
5	21-05-2026	Active site/Pocket Identification	Visualization of Protein structure	Uniprot, Pymol
6	21-05-2026	Homology Modeling	Concepts and Sequence search tool-BLAST	Selection of Template- Blast
7	22-05-2026	Homology Modeling	Validation of target structure	SwissPDBviewer, SAVES
8	22-05-2026	Ligand	Preparation of ligands	Drug bank, Pubchem
9	23-05-2026	Molecular Docking	Docking with Autodock and analysis	Autodock, Ligplot
10	25-05-2026	Types of CADD	SBDD, LBDD	Docking
11	26-05-2026	Pharmacophore & QSAR	Concepts	Zinc-Pharmer, Molinspiration
12	27-05-2026	Ligand Screening	Virtual Screening	Ligand databases
13	27-05-2026	ADMET	Pharmacokinetics & Pharmacodynamics	PreADMET
14	29-05-2026	Protein Motion	Conformational changes	VMD
16	30-05-2026	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	18/05/2026– 30/05/2026	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: 09 Faculty: Nil	External Participants count	Students: 02 Faculty: Nil

Report:

DST-FIST supported two weeks Internship on Computer Aided Drug Designing was organised by Research and Development Cell from 18/05/2026 till 30/05/2026. Around Eleven participants registered for the Internship. Both the theory and the practical sessions were handled by Dr. J. Lesitha Jeeva Kumari. The Internship 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 PubChem, PyMOL, SwissPDB Viewer,





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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 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/s9qTLRyE5PZkQncb7>

Feedback Summary:

The Computer Aided Drug Designing (CADD) workshop received highly positive feedback from all 11 participants, with 100% reporting that they were either satisfied or very satisfied with the program. Most participants agreed that the workshop objectives were successfully achieved, and the resource person effectively delivered both theoretical and practical aspects of the course. Participants appreciated the hands-on training, industry-relevant content, and the usefulness of CADD techniques for research and higher studies, with several recommending similar programs in the future.

Workshop Mentor

Associate Dean- Research

IQAC Director

Principal

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33 Years
of Educational
Excellence...

Research and Development Cell (RDC)

Programme Name: Internship

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

Date: 18-05-2026- 30-05-2026



Principa
Principal

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RESEARCH & DEVELOPMENT