MARUDHAR KESARI JAIN COLLEGE FOR WOMEN (AUTONOMOUS), VANIYAMBADI

(A Project of Sri Marudhar Kesari Jain Trust)

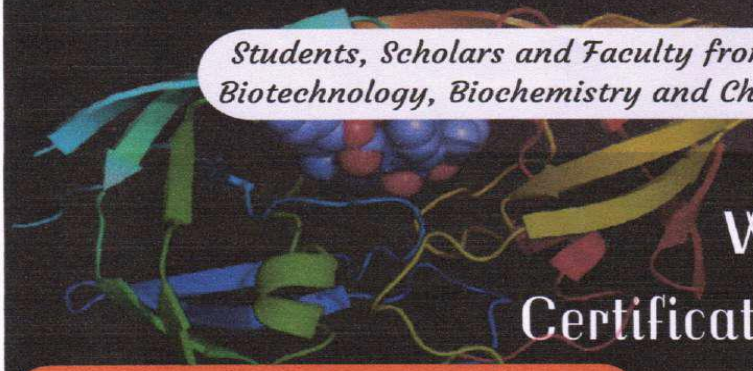
Recognised u/s 2(f) &12(B) by UGC Act, 1956 – Permanently Affiliated to Thiruvalluvar University– Accredited by NAAC with"A^{+}"Grade(4thCycle)–An ISO21001:2018 EOMS Certified Institution Supported by DST– FIST

RESEARCH AND DEVELOPMENT CELL ORGANIZED FIST- SUPPORTED WORKSHOP ON COMPUTER AIDED DRUG DESIGNING –16.12.2024

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

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 the disciplines of Biotechnology, Biochemistry and Chemistry are eligible



Workshop Kit and Certificate will be provided

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

REGISTRATION FEE

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

SCAN THE QR CODE TO REGISTER

or use the registration link
https://forms.gle/DfNWndpXe5vZCVqV8

For further details contact :
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Associate Dean-Research
Marudhar Kesari Jain College for Women, Vaniyambadi
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AGENDA

MARUDHAR KESARI JAIN COLLEGE FOR WOMEN,
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31 Years of Educational Excellence

FIST SUPPORTED WORKSHOP ON COMPUTER AIDED DRUG DESIGNING

Date: 16-12-2024 to 08-01-2025

Agenda

Day	Date	Topic	Theory Sessions	Practical Sessions
1	16-12-2024	Introduction to CADD	Overview of Computer aided drug design	-
2	17-12-2024	Bioinformatics for CADD	Databases for CADD	Databases- Pubmed, Uniprot, OMIM, PDB
3	18-12-2024	Types of CADD	Structure based drug design-Introduction	Literature study-Pubmed
4	19-12-2024	Drug Targets	Target Selection and Screening	Selection of Drug targets- Uniprot , PDB
5	20-12-2024	Active site/Pocket Identification	Visualization of Protein structure	Uniprot, Pymol
6	23-12-2024	Homology Modeling	Concepts and Sequence search tool-BLAST	Selection of Template-Blast
7	24-12-2024	Homology Modeling	Validation of target structure	SwissPDBviewer, SAVES
8	26-12-2024	Ligand	Preparation of ligands	Drug bank, Pubchem
9	27-12-2024	Molecular Docking	Docking with Autodock and analysis	Autodock, Ligplot
10	02-01-2025	Types of CADD	SBDD, LBDD	Docking
11	03-01-2025	Pharmacophore & QSAR	Concepts	Zinc-Pharmer, Molinspiration
12	04-01-2025	Ligand Screening	Virtual Screening	Ligand databases
13	06-01-2025	ADMET	Pharmacokinetics & Pharmacodynamics	PreADMET
14	07-01-2025	Protein Motion	Conformational changes	VMD
15	08-01-2025	Case study	Mucin-1 conformation analysis	VMD
16	09-01-2025	Valediction	Presentation by participants, Feedback and Distribution of Certificates	

10/01/25

RESEARCH & DEVELOPMENT

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MARUDHAR KESARI JAIN COLLEGE FOR WOMEN (AUTONOMOUS), VANIYAMBADI

RESEARCH AND DEVELOPMENT CELL ORGANIZED FIST- SUPPORTED WORKSHOP ON COMPUTER AIDED DRUG DESIGNING

–16.12.2024

REPORT

MARUDHAR KESARI JAIN COLLEGE FOR WOMEN, VANIYAMBADI
(A project of Sri Marudhar Kesari Jain Trust)

Activity Report

Title	FIST-Supported Workshop on Computer Aided Drug Designing			
Organized By	Research and Development Cell			
Type of Activity	Workshop			
Level	Institutional			
Date	16-12-2024	Time	1:30-3:40PM	
Venue	DST-FIST Lab	Mode	Offline	
Resource Person Details	Dr. J. Lesitha Jeeva Kumari, Research Associate, Department of Biotechnology			
Objective of the Programme	To provide a hands-on-training and impart theoretical knowledge on the various bioinformatics concepts, tools and software for theparticipants			
Internal Participants Count	39	**External Participants Count**	Nil	

The two weeks Internship on "Computer Aided drug designing" was organised by Research and Development Cell and conducted between 16-12-2024 to 08-01-2025. About 39 participants registered for the program. The theory and practical sessions were handled by Dr. R. Jesu Jaya Sudan and Dr. J. Lesitha Jeeva Kumari. This workshop provides hands-on-training on the major concepts in drug designing that includes Target selection, Ligand optimization, Pharmacokinetics, Pharmacodynamics, Virtual screening, Drug likeness, and Drug interaction. The program also covered different databases, tools and softwares like Pubchem, Pymol, SwissPDBviewer, Autodock vina, Ligplus, VMD, ADMET, SAVES, MolInspiration. The theoretical concepts of the 3-dimentional structures of proteins were elaborated and the participants were taught to visualize the protein structures and domains using various structure visualization programs like PYMOL, SwissPDBviewer.

The Program helps the Participants to understand the concepts and become familiar with the softwares and tools in drug designing. In addition, the participants gains insights in selecting ideal drug targets andto obtain practical skills to model and optimise ligands and were given the opportunity to visually observe the different methods of target inhibition and theoretically evaluate the drug likeness and its efficacy. At the end of every session the participants were given

assignment to carryout in their lab. On the final day the students were asked to present the collective report of their findings and explain the inferences. During the valediction day the students were asked to give the feedback and the workshop ended with Certificate distribution.

Outcome of the Programme

The particpants 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

10/01/25

Head/ Co Ordinator

10/1/25

Director-IQAC

Principal

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PHOTOS

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