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(AUTONOMOUS)

VANIYAMBADI, TIRUPATTUR DT – 635 751

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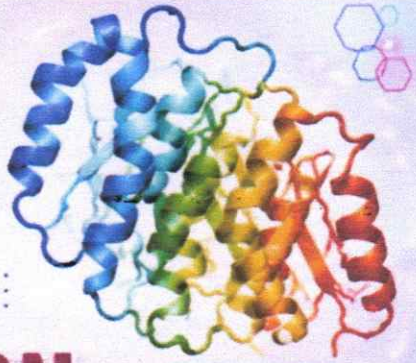
PG & Research Department of Biochemistry

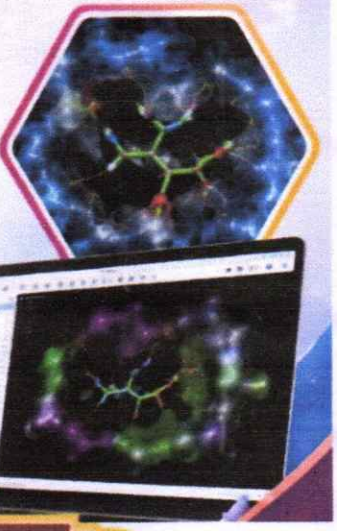
Organizes

MoU Activity

Hands-on Training Programme on

PROTEIN STRUCTURE PREDICTION and MOLECULAR DOCKING.





LEARN Cutting-edge Tools and Techniques

EXPLORE Protein Structure Prediction

PERFORM Molecular Docking Simulations

APPLY In Drug Discovery & Research

ANALYZE Results with Confidence

Supported by DBT STAR College Scheme

Date : 22.08.2026 | Time : 10.00 am | Venue : Sri Arihanth Seminar Hall

CHIEF GUESTS

Dr. I. Ancy
Research Scientist - Bioinformatics
Bioinnov Solutions LLP

Ms. V. B. Swethaa
Senior Researcher
Bioinnov Solutions LLP

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

Sri. V. Dilip Kumar Jain | Sri. Anand Singhvi | Dr. M. Inbavalli | Ms. R. Malarkodi

MARUDHAR KESARI JAIN COLLEGE FOR WOMEN (AUTONOMOUS)
VANIYAMBADI

PG & RESEARCH DEPARTMENT OF BIOCHEMISTRY
Organizes
MoU Activity
Hands-on Training Programme
on
Protein Structure Prediction & Molecular Docking
Supported by DBT STAR College Scheme

AGENDA

Date: 22.08.2026

Venue: Sri Arihanth Seminar Hall **Time: 10.00 A.M**

- **Prayer**
- **Welcome Address** : **Ms. K. Vishnu Priya III B.Sc Biochemistry**
- **Felicitation** : **Dr.M.Inbavalli, Principal,MKJC**
- **Guest Introduction I** : **Ms V. Thulasi –III B.Sc Biochemistry**
- **Guest Introduction II** : **Ms A.Dharshini -III B.Sc Biochemistry**
- **Honoring the Chief Guest** : **Dr.M.Inbavalli, Principal, MKJC**
- **Speaker I** : **Dr. I. Ancy**
  Research Scientist - Bioinformatics
  Bioinnov Solutions LLP, Salem
- **Speaker I** : **Ms V.B. Swethaa**
  Senior Researcher
  Bioinnov Solutions LLP, Salem
- **Vote of thanks** : **Ms. S.Arvitha –III B.Sc Biochemistry**
- **National Anthem**
-

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Activity Report

Hands-on Training Programme on Protein Structure Prediction and Molecular Docking

Input

The PG & Research Department of Biochemistry organised a Hands-on Training Programme on Protein Structure Prediction and Molecular Docking as part of its MoU activity, supported by the DBT STAR College Scheme. The programme was designed to provide students with exposure to contemporary computational biology and bioinformatics approaches used in drug discovery and biomedical research.The programme combined expert lectures with practical training, enabling students to understand the relevance of computational methods in modern pharmaceutical research and gain introductory practical experience with commonly used bioinformatics and molecular modelling tools.bioinformatics and molecular modelling tools.

Objectives of the Programme

The major objectives of the programme were to:

- Introduce students to the scope and applications of computational biology and bioinformatics.
- Familiarise students with current approaches in drug discovery and precision medicine.
- Familiarise students with tools such as MGL Tools, AutoDock 4, PyMOL and PLIP.
- Provide an overview of protein structure prediction and docking.
- Provide practical exposure to AlphaFold and protein structure databases.
- Develop basic practical skills in molecular docking and docking workflow.
- Bridge theoretical learning with practical applications in pharmaceutical and biomedical research.

Process

Session I – Expert Lecture on Computational Biology

The morning session was handled by **Dr. I. Ancy**, Research Scientist – Bioinformatics, Bioinnov Solutions LLP. She introduced the students to the growing importance of computational biology in the global pharmaceutical sector and highlighted emerging opportunities in bioinformatics-driven research.

The session provided an overview of the future applications of precision medicine through network pharmacology and explained how computational approaches are increasingly integrated into drug discovery. The discussion covered major stages of the drug discovery

The discussion covered major stages of the drug discovery process, including protein structure determination, compound screening, drug selection, lead optimisation and molecular docking.The expert interaction helped students understand how computational methods can support the identification and evaluation of potential drug candidates and contribute to faster and more informed decision-making in pharmaceutical research.

Session II – Hands-on Training on Protein Structure Prediction

The second session was handled by **Ms. V. B. Swethaa**, Senior Researcher, Bioinnov Solutions LLP. The students were provided with practical exposure to AlphaFold-based protein structure prediction and the use of protein databases.

The hands-on session enabled students to understand the basic workflow involved in obtaining and interpreting predicted protein structures and accessing relevant structural information from databases. The activity gave students an opportunity to relate protein structure concepts learned in their academic curriculum with current computational tools used in research.

Session III – Hands-on Training on Molecular Docking

The afternoon practical session was conducted by **Dr. I. Ancy** and focused on the fundamentals of molecular docking and structure-based drug discovery.

Students were introduced to the use of MGL Tools and AutoDock 4 for carrying out docking studies. The training covered the overall docking workflow, including target selection, ligand preparation, grid selection, docking simulation and analysis of docking results.

The students were also introduced to PyMOL for structural visualisation and PLIP (Protein–Ligand Interaction Profiler) for analysing protein–ligand interactions, visualization by**Ms. V. B. Swethaa**. The practical exposure helped students understand how docking results can be visualised and interpreted in the context of molecular interactions.

Output

- A one-day hands-on training programme was conducted on Protein Structure Prediction and Molecular Docking.
- Two external experts from Bioinnov Solutions LLP served as resource persons.
- Expert sessions on computational biology, precision medicine, network pharmacology and drug discovery were conducted.
- Practical sessions on AlphaFold, protein databases, MGL Tools, AutoDock 4, PyMOL and PLIP were conducted.
- Hands-on training covered the basic molecular docking workflow from target selection to analysis and visualisation.
- Students participated in lecture, demonstration and hands-on practical sessions.

This programme can be mapped primarily to SDG 4 – Quality Education, SDG 3 – Good Health and Well-being, SDG 9 – Industry, Innovation and Infrastructure, SDG 17 – Partnerships for the Goals.

Outcome

- Students developed an understanding of the role of computational biology in drug discovery.
- Students acquired basic practical skills in protein structure prediction using AlphaFold.
- Students developed familiarity with molecular docking and protein–ligand interaction analysis.
- Students improved their ability to understand the target selection, ligand preparation, grid selection, docking and analysis workflow.
- Students gained introductory competency in using MGL Tools, AutoDock 4, PyMOL and PLIP.
- Students developed greater awareness of precision medicine, network pharmacology and research opportunities in bioinformatics.

The programme successfully provided students with an opportunity to connect their theoretical knowledge in biochemistry with emerging computational and bioinformatics applications. The combination of expert interaction and hands-on training strengthened students' awareness of current research practices in protein structure analysis and drug discovery.The practical sessions also encouraged students to explore computational tools and develop an interest in interdisciplinary research involving biochemistry, bioinformatics, molecular biology and pharmaceutical sciences.

for M.R 29/8/26
Head of the Department

28/8/26
Dean

29/08/2026
IQAC Director

Principal

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MARUDHAR KESARI JAIN

College for Women (Autonomous), Vaniyambadi

33 Years of Educational Excellence...

Topic: Hands-on Training Programme on Protein Structure Prediction and Molecular Docking

Date : 22.08.2026

Organized by: PG & Research Department of Biochemistry

Venue: Marudhar Kesari Jain College for Women (Autonomous), Vaniyambadi

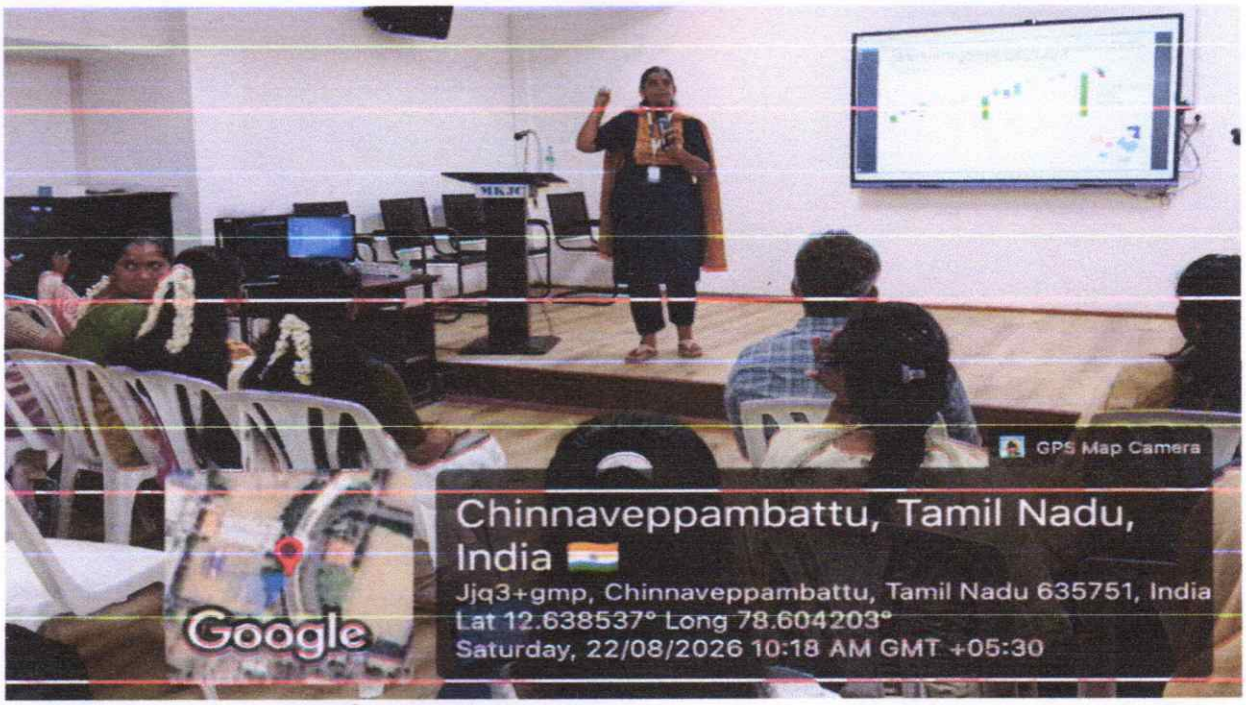
Time: 10.00 a.m. to 3.00 pm

Venue: Sri Arihanth Seminar Hall

Activity: MoU Activity

Support: DBT STAR College Scheme

Geotag Photos



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