Aarupadai Veedu Institute of Technology

Vinayaka Mission's Research Foundation

Department of Biotechnology

Report of Hands on Training on Next generation AI tool in Bioinformatics

15.9.2025 and 16.9.2025

Department of Biotechnology, AVIT organized the **Hands on Training on Next generation AI tool in Bioinformatics on 15.9.2025 and 16.9.2025**. The session started at 9.30 AM on 15.09.25 the gathering was welcomed by Dr.Nirmala. A, Associate Professor and Head, Department of Biotechnology, AVIT which was followed by the speaker introduction by, Dr.L.Nagarajan, Associate Professor, Department of Biotechnology. Followed by handing over the session to guest speaker Mr.KK. Prasanth, Founder and CEO Simbioen labs, Chennai.

He started the session by giving the objectives of this program to understand the evolution of bioinformatics and the role of AI and explore how next-generation AI is transforming life science research. Bioinformatics traditionally focused on computational biology, genome analysis, and molecular data processing. With rapid advances in AI, deep learning, and generative models, new tools can now predict protein structures, Design new drugs, interpret massive genomic datasets, automate data curation and analysis and enabling personalized medicine.

Era	**Approach**	**Key Features**
1.0 – Classical Bioinformatics	Sequence alignment, BLAST, phylogenetics	Rule-based, algorithmic

2.0 – Machine Learning	SVM, Random Forest, clustering	Feature engineering, predictive models
3.0 – Deep Learning	CNNs, RNNs, Transformers	End-to-end prediction, structure modeling
4.0 – Generative AI (Next-Gen)	LLMs, diffusion models, multi-modal AI	Drug design, protein generation, knowledge synthesis

Hands on training focused on the following topics given in the schedule (Table -1). On the day-1 morning session training focused on explore the role of computational tools in drug design, development and safety assessment. It covered the data source cheminformatics techniques, and the importance of integrating pharmacological and toxicological data. Focused on understanding how physicochemical properties influence drug behavior and interaction. Demonstrated the use of predictive models for bioactivity, ADME (Adsorption, distribution, metabolism and excretion) and drug interaction analysis. Discussed methods for identifying potential biological targets for drug using computation approaches, included ligand based and structure based target prediction techniques. In afternoon session, explored how artificial intelligence accelerate drug discovery processes. Resource person explained about AI driven data analysis, virtual screening, and predictive modelling and also focused on docking workflow, scoring function and validation. Practical demonstration includes, ligand identification, target selection, ADME study etc.,

Table-1 TRAINING SCHEDULE

NEXT- GENERATION AI TOOLS IN BIOINFORMATICS			
DAY	**Session**	**Session Topic**	**Session Details**
	09.00 - 10.15	Introduction to Pharmacoinformatics & Toxicoinformatics	PPT & Online servers and Structural alerts
	Break		

Day-1	10.15 - 12.30	Drug Interactions - Physiochemical property and Bioactivity predictions	Marvin, Chemdraw, Swiss ADME, Pass Online, CLC Pred, GUSAR, ADMET 2.0, CODD-PRED
	Break		
	01.15 - 02.00	Introduction to Genomics, Target Predictions	Gene bank, Super Pred, BD, Swiss Target Prediction
	Break - 2		
	02.00 – 03.30	Introduction to Proteomics and Protein Structure Modelling	Uniprot, PDB, Swiss Modeller, Protoparam, Phyre2
Day-2	09.00 - 10.15	Role of AI in Drug Discovery Introduction to Docking	PPT
	Break		
	10.15 - 12.30	Preparation for Molecular Docking	Marvin Sketch, Pymol, Avogadro
	Break		
	01.15 - 02.00	Docking, Clustering and Pose Generation	Auto Dock and Auto grid, MGL Tools
	Break - 2		
	02.00 – 03.30	Visualization And Result Interpretation	Chimera, Pymol, Discovery studio Visualizer

On the second day, focused on steps to prepare both ligand and receptors structure, protein cleaning, ligand preparation, identifying active site, discussed methods to analyze multiple docking process. Focused on visualizing docking results on understanding ligand receptor interaction, usage of tools like PyMOL, Chimera, Avogadro, Auto Dock and Auto grid, MGL Tools ect., Resource person focused on visualizing docking result to understand ligand –receptor interaction.


GPS Map Camera
Pattipulam, Tamil Nadu, India
M54h+hm8, Pattipulam, Tamil Nadu 603104, India
Lat 12.656567° Long 80.179304°
15/09/2025 01:27 PM GMT +05:30
Google


GPS Map Camera
Pattipulam, Tamil Nadu, India
M54h+hm8, Pattipulam, Tamil Nadu 603104, India
Lat 12.656563° Long 80.179316°
15/09/2025 01:32 PM GMT +05:30
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This also created entrepreneurial skill to start their own firm by carrying out all the basic level of research before entering into this field. On the whole around 60 students were benefited from this session. Finally the session was closed on 16.09.25 afternoon 4:40 p.m with a vote of thanks delivered by Ms.Devi Sai Prasanna , III year, Department of Biotechnology, AVIT.