



2 DAYS WORKSHOP ON

AI IN BIOINFORMATICS AND DRUG DISCOVERY

BY TECH BOOSTER

JOIN NOW AND TAKE A STEP TOWARDS YOUR DREAM CAREER



DAY 1 – Decoding Life with Data

SESSION 1: The AI Revolution in Biology & Medicine

◆ Why Traditional Drug Discovery Takes 10–15 Years?

Cost & failure rates

Clinical trial challenges

◆ How AI is Changing Healthcare

Faster drug screening

Disease prediction

Personalized medicine

◆ Real Industry Case Studies

AI-designed molecules

AlphaFold breakthrough

AI in vaccine development

Activity:

Students map traditional vs AI-driven drug discovery timeline.

SESSION 2: Bioinformatics Essentials (Hands-On)

◆ Biological Databases

NCBI

UniProt

PDB

PubChem

◆ Sequence Retrieval & Formats

FASTA

GenBank

◆ Practical:

Retrieve a gene sequence

Run BLAST analysis

Interpret similarity results

Outcome: Students perform their first real biological data analysis.



SESSION 3: Introduction to AI & Machine Learning

◆ ML Concepts Made Simple

Supervised Learning

Classification vs Regression

Clustering

◆ Biological Use Cases

Toxicity prediction

Disease classification

Gene expression analysis

Hands-on:

Basic ML demo in Google Colab

Simple classification example

SESSION 4: Protein Structure & AI

◆ Why Protein Structure Matters in Drug Discovery

◆ AlphaFold & Structure Prediction

◆ Visualization using:

PyMOL / Online viewers

Practical:

Students visualize a protein and identify active site regions.

SESSION 5: AI in Drug Discovery Pipeline

◆ Target Identification

Genomics data

Network biology

◆ Virtual Screening

Structure-based design

Ligand-based design

◆ De Novo Drug Design

Generative AI concept

VAEs & GANs (conceptual overview)

Activity:

Students screen mock compounds dataset.

SESSION 6: ADMET & Drug Safety Prediction

◆ What is ADMET?

Absorption

Distribution

Metabolism

Excretion

Toxicity

◆ AI in Toxicity Prediction

◆ Drug-Drug Interaction Prediction

Hands-on:

Predict basic molecular property using dataset demo.



CONTENTS Day2 Contd.



SESSION 7: AI in Clinical Trials & Personalized Medicine

- ◆ **AI in Patient Recruitment**
- ◆ **Biomarker-based trials**
- ◆ **Outcome prediction models**

Case Study Discussion:

“Would this drug pass Phase 3 trial?”

🎓 SESSION 8: Mini Capstone Project

Students choose one:

Sequence Analysis Project

Build a simple ML classifier

Target prediction exercise

ADMET prediction mini model

Presentation + Certificate Distribution