biotecnika
Your Bio Resource

AI ML in Drug Discovery, Bio-Pharma, Cheminformatics Hands-on Training Program

WORK IN PROJECTS |
PUBLISH PAPERS |
GET WORK EXPERIENCE
in AI ML

With 100% Placement Assistance

Extensive 45 Days Hands-on Training With 3,6 & 12 Months Project Work

Mail: info@biotecnika.org

stores.biotecnika.org

Why Join This Training?

- Expert-Led Instruction: Learn from industry leaders and academic experts.
- Hands-On Experience: Practical training on tools like TensorFlow, RDKit, and KNIME.
- Real-World Applications: Solve challenges in drug discovery, molecular design, and personalized medicine.
- Flexible Learning Paths: Choose from 3, 6, or 12-month LIVE project work.

Why Learn AI/ML in Biopharma & Chemistry?

- Stay ahead in the fast-evolving pharmaceutical industry.
- Build high-demand skills across AI, ML, and cheminformatics.
- Contribute to cutting-edge research and drug development.

Toll Free - 1800-1200-1818

www.Biotecnika.org

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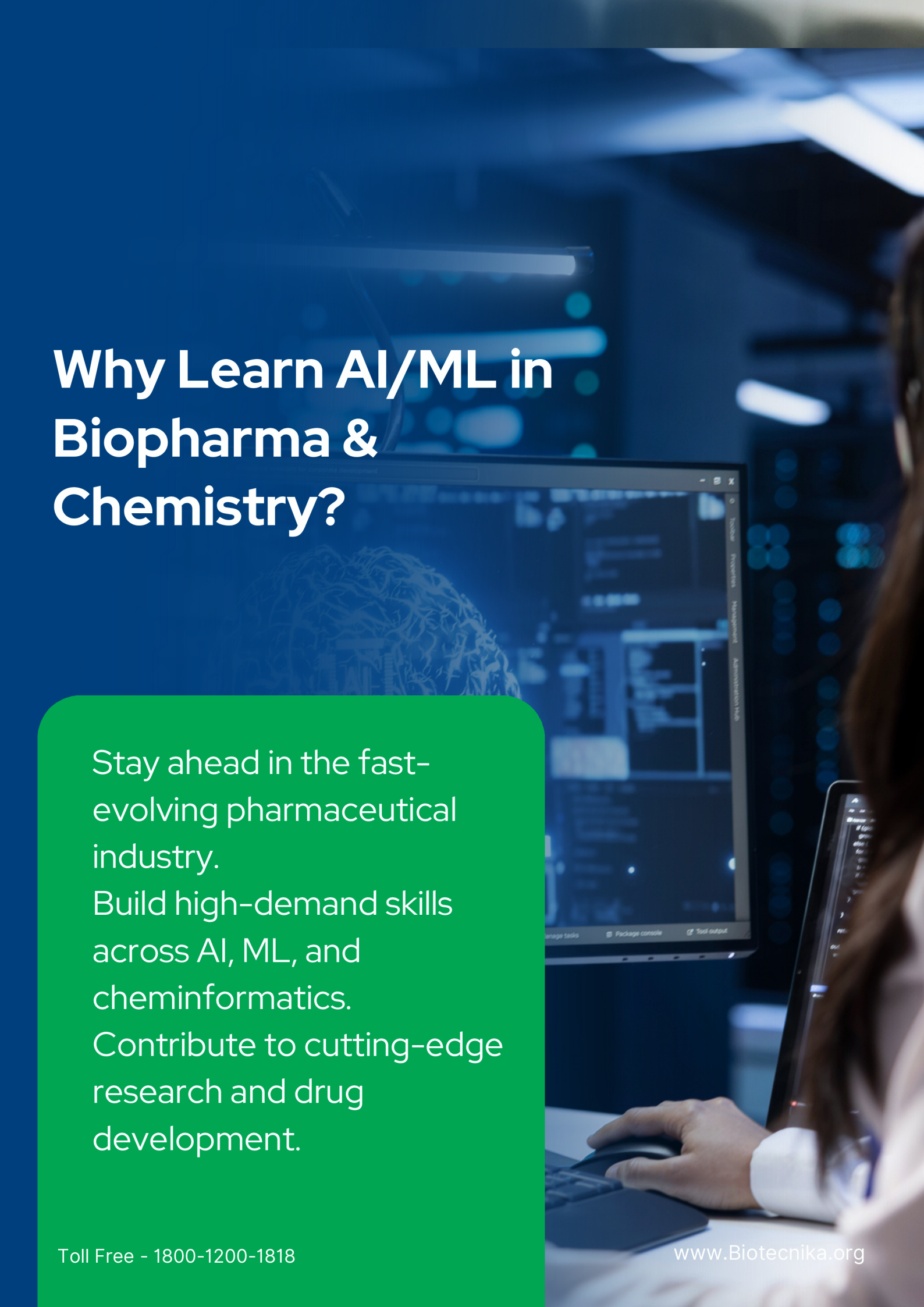

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Course Curriculum

Week 1: Foundations of Drug Discovery

- **Day 1:** Introduction to the Drug Discovery Pipeline – Target Identification → Screening → Optimization → Preclinical
- **Day 2:** Role of Bioinformatics & Cheminformatics – Ligand-based vs Structure-based methods
- **Day 3:** Molecular Representations – SMILES, InChI, SDF, FASTA formats
- **Day 4:** Visualization of Molecules – Tools: RDKit, PyMOL demo
- **Day 5:** Introduction to Drug Databases – DrugBank, ChEMBL, BindingDB, PubChem
- **Day 6:** Understanding Bioactivity Metrics – IC50, EC50, Ki and their usage in modeling

Course Curriculum

Week 1: Foundations of Drug Discovery

- **Day 7:** Target Identification & Validation – Omics data to gene prioritization (GEO, DisGeNET)
- **Day 8:** Molecular Docking & Virtual Screening – Concepts & tools overview
- **Day 9:** Lead Optimization & Drug Repurposing – Lipinski's Rule, ADMET considerations

Week 2: ML Foundations & Python for Drug Discovery

- **Day 10:** Python Basics – Data types, functions, pandas, numpy
- **Day 11:** Visualizing Drug Data – matplotlib, seaborn for bioactivity & chemical structure

- **Day 12:** Introduction to Machine Learning – Supervised vs Unsupervised, ML pipeline
- **Day 13:** Data Preprocessing – Cleaning, scaling, encoding SMILES
- **Day 14:** Feature Extraction – RDKit descriptors, molecular fingerprints
- **Day 15:** ML Models I – Classification: Logistic Regression, Decision Trees, Random Forest
- **Day 16:** ML Models II – Regression: Linear Regression, Ridge, SVR
- **Day 17:** Model Evaluation – Confusion Matrix, ROC-AUC, MAE, RMSE
- **Day 18:** Case Study – Classify drug-like vs non-drug-like molecules

Course Curriculum

Week 3: QSAR, Pharmacophore Modeling & Bioactivity Prediction

- **Day 19:** Introduction to QSAR – Concepts & datasets
- **Day 20:** Building Regression Models – IC50 prediction
- **Day 21:** Model Tuning – GridSearchCV, Cross-validation
- **Day 22:** AI in COVID-19 Drug Discovery – Predicting SARS-CoV-2 Inhibitor Activity
- **Day 23:** Unsupervised Learning – K-Means, DBSCAN
- **Day 24:** Dimensionality Reduction – PCA, t-SNE; Case study: clustering molecules
- **Day 25:** AI in Pharmacophore Modeling

Course Curriculum

Week 3: QSAR, Pharmacophore Modeling & Bioactivity Prediction

- **Day 26:** Drug Repurposing – Similarity-Based Clustering
- **Day 27:** Case Study – End-to-End Bioactivity Prediction Pipeline

Week 4: Deep Learning for Drug Discovery

- **Day 28:** Introduction to Deep Learning – Concepts and terminologies
- **Day 29:** Keras & PyTorch – Intro for molecular data
- **Day 30:** CNNs & RNNs – For SMILES sequences
- **Day 31:** Autoencoders – For molecular representation

Course Curriculum

- **Day 32:** Generative Models – VAE & GAN; Case study: generate molecules
- **Day 33:** Graph Neural Networks – For molecule structure
- **Day 34:** DeepDTA – Protein-ligand binding affinity prediction
- **Day 35:** Case Study – Toxicity prediction with deep learning

Week 5: Integrative AI Applications & Current Trends

- **Day 36:** Chemoinformatics for Natural Products
- **Day 37:** NLP in Drug Discovery – Literature mining, NER with PubMed

Course Curriculum

- **Day 38:** Reinforcement Learning – Drug optimization & reward modeling
- **Day 39:** ADMET Property Prediction – Blood-brain barrier, hERG toxicity, etc.
- **Day 40:** AI in Docking & MD Simulations – Integration overview, ML-based binding score prediction
- **Day 41:** Building ML Pipeline – End-to-end model, deployment with Streamlit
- **Day 42:** AI in Personalized Medicine & Healthcare
- **Day 43:** Regulatory Guidelines & Ethics – Bias, explainability, validation, clinical risk
- **Day 44:** Current Trends – Career guidance & Capstone project discussion
- **Day 45:** Open Doubt-Solving & Discussion Session

Project Work Options

3 Months

Short-term projects focusing on specific applications like QSAR modelling or molecular docking.

6 Months

Intermediate projects involving more complex models and integration with real-world datasets.

12 Months

Long-term research projects aiming at publication-quality results or industrial application.

Project Topics
for AI & ML in Chemistry and Bio-Pharma

- Prediction of Drug-Likeness Using Machine Learning on Molecular Descriptors – 6 months
- In Silico Screening of Natural Compounds for Anti-Cancer Activity – 6 months
- Cheminformatic Approaches for Drug Design and Drug Discovery – 6 months
- Virtual Screening of Potential Inhibitors for SARS-CoV-2 Main Protease – 6 months
- Virtual Screening of Potential Inhibitors for SARS-CoV-2 Mpox – 6 months
- Molecular Docking and Machine Learning-Based Analysis of Anti-Inflammatory Compounds – 3 months
- Molecular Docking and Machine Learning-Based Analysis of Antiviral Compounds – 6 months

Project Topics
for AI & ML in Chemistry and Bio-Pharma

- Exploring the Use of Deep Learning for Predicting Toxicity in Chemical Compounds – 6 months
- Machine Learning Based Screening of Curcuma longa for Drug Discovery – 6 months
- Application of Neural Networks in Predicting the Solubility of Pharmaceutical Compounds – 6 months
- AI-Driven Prediction of Drug-Target Interactions for New Chemical Entities – 6 months
- Computational Prediction of Binding Affinity for Enzyme-Substrate Interactions – 6 months
- AI-Assisted Designing of Novel Anticancer Compounds – 6 months
- Application of AI in the Prediction of Protein-Ligand Binding Sites – 6 months
- Virtual Screening and Docking Studies of Phytochemicals Against Cancer Targets – 6 months

Project Topics
for AI & ML in Chemistry and Bio-Pharma

- AI/ML-Assisted Molecular Modelling Studies for Protein Stability Analysis – 6 months
- Prediction of Protein Secondary Structure Using Basic Supervised Learning Algorithms – 6 months
- Cheminformatics Approaches to Predict the Reactivity of Organic Compounds – 6 months
- AI-Assisted Approaches for Structure-Based Drug Design 6 months
- AI-Assisted Approaches for Ligand-Based Drug Design 6 months
- Machine Learning Models for Predicting Drug Side Effects Based on Chemical Structure 6 months
- Predictive Modeling of Drug Permeability Using AI Techniques 6 months
- Molecular Docking for HIV Inhibitor Screening (Bioinformatics, AI/ML in Drug Discovery) – 3 months

Project Topics
for AI & ML in Chemistry and Bio-Pharma

- Host-Pathogen Interaction Modeling for HIV (Bioinformatics, AI/ML in Drug Discovery) – 6 months
- Network-Based Drug Repurposing for HIV (Bioinformatics, AI/ML in Drug Discovery) – 6 months
- Meta-Learning Framework for Bioactivity Prediction on Low-Data Orphan Targets Using Neural Processes – 12 months
- Explainable AI (XAI) for Toxicity/ADMET Predictions – 3 months
- Unifying Transcriptomics & Chemoinformatics for Personalized Drug Repurposing – 6 months
- Explainable AI for ADMET Prediction Using Multi-Modal Data 3 months
- Machine Learning-Based Virtual Screening of Natural Compounds for Antibacterial Activity (Proteases) – 3 months

Project Topics
for AI & ML in Chemistry and Bio-Pharma

- Predictive Modeling and Lead Optimization for Anticancer Agents Using AI – 6 months
- Deep Learning Framework for Structure-Based Drug Design Targeting Viral Proteins – 12 months
- Reinforcement Learning-Based Drug Design Against Kinase Targets – 6 months
- AI-Based QSAR Modeling for Anti-Cancer Drug Lead Optimization – 12 months
- Deep Learning for Promoter Region Prediction: Use CNNs (in Keras/TensorFlow) to Detect Promoter Regions in Genomic DNA – 6 months
- Transfer Learning for Cross-Species Drug Repurposing – 6 months

Top Companies Hiring in AI/ML Drug Discovery & Cheminformatics

Pharma & Biotech

- NOVARTIS
- AstraZeneca
- GSK
- Pfizer
- sanofi
- Roche
- Biocon
- Syngene

AI & Data Science

- NVIDIA
- DeepMind
- IBM Research
- Microsoft AI
- OpenAI
- Benevolent AI
- Atomwise
- Insilico Medicine

Consulting & R&D Labs

- TCS
- accenture
- IQVIA
- cognizant
- Glenmark — A new way for a new world
- ZS
- Dr. Reddy's
- wipro

Career Opportunities After Training

Completing this program opens doors to a wide range of career paths across the pharmaceutical, biotechnology, healthcare, and AI industries. Some of the top roles you can pursue include:

Career Opportunities After Training

AI/ML Drug Discovery Specialist

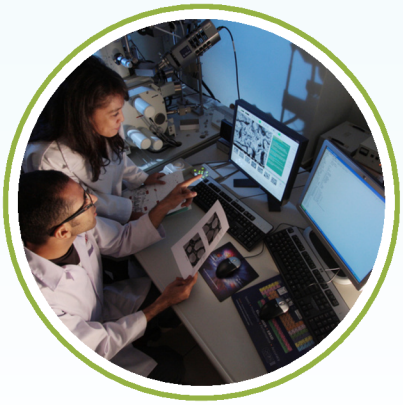
Work with pharmaceutical companies and research labs to develop AI models that accelerate drug development pipelines

Cheminformatics Scientist

Design, manage, and analyze chemical databases, and use computational methods to aid drug design and discovery

Bioinformatics Analyst:

Interpret biological data using computational tools, especially in genomics, transcriptomics, and proteomics



Computational Chemist

Use molecular modeling, simulations, and quantum chemistry tools to understand and predict molecular behavior.

Career Opportunities After Training

Data Scientist – Pharma Domain:

Analyze clinical, chemical, and biological data to derive insights for R&D, drug efficacy, and safety

Research Associate

AI in Biotech: Contribute to ongoing research using AI/ML models to solve problems in biotechnology and healthcare

Molecular Modelling & Simulation Expert

Create virtual molecular environments to study interactions and optimize lead compounds

Clinical Data Scientist

Design and evaluate statistical models that support clinical trials, patient stratification, and personalized medicine.

Career Opportunities After Training

Pharmaceutical R&D Analyst:

Evaluate market trends, R&D productivity, and competitor strategies to support drug development and commercialization decisions

These roles span academia, industry, startups, contract research organizations (CROs), and healthcare AI companies—making this program a versatile launchpad for your scientific career.

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Equip yourself with industry-ready AI/ML skills for pharma and chemistry innovation. Whether you're upskilling or transitioning careers—this program is your gateway to a future in drug discovery research and innovation.

Enroll Today!

About the Instructor

Ms Snigdha Tiwari

Clinical Research & Bioinformatics Trainer | Expert in Computational Biology, Telemedicine & Data-Driven Healthcare

Snigdha Tiwari is an accomplished Senior Research Fellow from IIT Roorkee, bringing over five years of multidisciplinary experience in computational biology, bioinformatics, and clinical research systems. With a strong foundation in healthcare data management and translational research, she has successfully led multiple collaborative projects with premier institutes like AIIMS Delhi and THSTI Faridabad.

Her key contributions include the design and deployment of the UTSARJAN App, a pioneering telemedicine solution for pediatric nephrotic syndrome data collection, now publicly available via the Play Store. She has in-depth experience in molecular docking, protein-protein and protein-ligand interactions, and molecular dynamics simulations using advanced tools such as GROMACS, PyMol, Chimera, and Discovery Studio.
Currently pursuing her PhD in Computational Biology, Snigdha brings a rare blend of bioinformatics expertise, clinical data insights, and digital health innovation. She is passionate about training the next generation of life science professionals and equipping them with practical skills in clinical research, healthcare informatics, and regulatory-compliant data handling.

At Biotecnika, she will mentor and guide students through real-world clinical research workflows, data interpretation techniques, and hands-on project work to help them become job-ready clinical research professionals.

About the Instructor

Dr. Elamathi

ALML & Bioinformatics Scientist

Dr. Elamathi Natarajan is a dedicated bioinformatician with a robust background in computational biology, data analysis, and genomics. Holding a Doctorate in Bioinformatics from Dr. A.P.J Abdul Kalam Technical University and an MBA in Information Systems Management, she has made significant contributions to the field through both research and teaching.

she has served as an Assistant Professor and Head of Department (HOD) In-Charge at Kalinga University, Raipur, where she excelled in lecturing, research, and departmental management. At Biotecnika Info Labs Pvt Ltd, Bangalore, she played a key role in academic support, enhancing student success through coaching and program development.

Elamathi's expertise includes developing bioinformatics pipelines, conducting quality assessments, and applying machine learning algorithms to genomics data.

Recognized for her work, including a Senior Research Fellowship from the Indian Council of Medical Research (ICMR), she continues to drive innovation in bioinformatics and is seeking a new challenge to further advance scientific discoveries.

About the Instructor

Mr.Prodyot Banerjee

CADD, Bioinformatics & Genomics Scientist

Prodyot Banerjee is a seasoned professional in Computer-Aided Drug Designing, Bioinformatics Analysis, and Genomics, boasting rich experience from institutions like CSIR-IGIB, CSIR-CLRI, IIT Madras, and Delhi Technological University.

With an M.Tech in Bioinformatics from Delhi Technological University, Prodyot has excelled in research and development roles, presenting his work at prestigious venues like IIT Kharagpur. His research is published in esteemed journals such as IEEE and Frontiers in Pharmacology, with more underway. Prodyot's GATE 2019 qualification from IIT Madras underscores his dedication to both academic excellence and professional growth. With a proven track record and relentless pursuit of knowledge, he is a valuable asset in bioinformatics, genomics, and computer-aided drug design endeavors.

About the Instructor

Dr. Nilofer K Shaikh

Bioinformatics global Scientist, Biotecnika

With a strong background in big data analysis using computational approaches in cancer omics data, Ms. Nilofer K Shaikh brings a wealth of experience from MIT ADT University. Her expertise spans cancer research, drug design, molecular dynamics simulation, data mining, and various omics technologies. Proficient in Python, R, and computational methodologies, she has a deep understanding of genomics, metabolomics, proteomics, transcriptomics, pharmacogenomics, and AI for cancer treatment. Her skillset also includes machine learning, MySQL database management, and natural language processing (NLP).

About the Instructor

Dr. Neeraj Kumar (BioIT Departme

Clinical Research Professional
Clinical Research Trainer at Biotecnika

Dr. Neeraj Kumar is a computational biologist and bioinformatician with expertise in AI-driven drug discovery, cheminformatics, and structural bioinformatics. He holds a Ph.D. inBioinformatics from CSIR-IHBT and AcSIR, India, specializing in machine learning (ML) and deep learning (DL) for virtual screening, drug repositioning, and lead optimization. His postdoctoral research at Pennsylvania State University focused on developing computational algorithms for immunoglobulin analysis. He obtained extensive experience in ML/DL frameworks (TensorFlow, PyTorch), cheminformatics (RDKit, OpenBabel), and molecular modelling (AlphaFold, Rosetta, GROMACS) and has contributed primarily to AI- guided virtual screening pipeline development and HIV drug discovery and structural bioinformatics projects. His research work has been published in esteemed journalsincluding Journal of Cheminformatics, Medicinal Research Reviews, Computer in Biology and Medicine, with more in progress. He has also qualified prestigious national-level exams including UGC-NET, GPAT, NIPER-JEE, and GATE.


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