

Toxicology & Computational Biology Internship Programme

1. Programme Overview

This internship is designed as a curriculum-mandated, credit-bearing programme for third-year Bachelor's students in Molecular Biology, Toxicology, allied Life Sciences/Pharmacology streams or B. Tech Biotech, Food tech students. It bridges two pillars that define a modern skill set: (a) the regulatory and risk-assessment framework that governs how chemicals and drugs are legally tested and approved, and (b) the AI/computational toolset that is rapidly transforming molecular biology, drug discovery, and predictive toxicology. The programme closes with a real-world field immersion in forensic toxicology.

Parameter	Detail
Duration	6 weeks
Frequency	2 days per week
Contact hours/day	3 hours
Total contact hours	36 hours
Credits	4 (as per curriculum requirement)
Eligibility	3rd Year B.Sc./B. Tech Toxicology, allied Life Sciences students
Mode	In-house computational lab sessions + external field visit
Prerequisites	Basic cell biology & biochemistry; no prior coding experience required

1.1 Programme Objectives

- Build working familiarity with the international regulatory framework (OECD, ICH) that governs chemical and drug safety testing.
- Introduce New Approach Methodologies (NAMs) and the 3Rs principle as the modern, animal-free direction of toxicology testing.
- Give hands-on exposure to virtual toxicology laboratories where real wet-lab experiments cannot be performed within the internship timeframe.
- Build a working, tool-based understanding of how AI and computational methods (structure prediction, docking, network biology) are used in modern drug discovery and toxicological risk prediction.
- Introduce statistical analysis and AI-assisted research skills relevant to a final-year research project or dissertation.
- Provide direct field exposure to applied/forensic toxicology through a hospital-based visit.

1.2 Learning Outcomes

By the end of this internship, a student will be able to:

- Explain the roles of OECD Test Guidelines, ICH guidelines, and NAMs in chemical/drug safety assessment.
- Apply the 3Rs principle to critically evaluate a testing strategy for reduction of animal use.
- Run a virtual toxicology experiment and interpret its output.
- Retrieve a protein structure from the PDB and visualise/analyse it in PyMOL.
- Perform a basic receptor-ligand docking study using AutoDock Vina and interpret binding affinity scores.
- Generate and compare AI-predicted protein structures (AlphaFold3, ESMFold) against experimental structures.
- Use a generative docking model (DiffDock-L) and predict ADMET properties of a candidate molecule.

- Construct and interpret a protein-protein interaction network (STRING/Cytoscape) and map genes to biological pathways (KEGG/DAVID).
- Design, execute, and statistically analyse (GraphPad Prism) a small computational toxicology mini-project, and present it clearly.
- Describe how forensic toxicology is practised in a real clinical/medico-legal setting.

2. Programme Structure

Week	Day	Module	Session Focus	Format
1	Day 1	A - Regulatory Toxicology	OECD Guidelines & Global Regulatory Bodies	Theory + Discussion
1	Day 2	A - Regulatory Toxicology	ICH Guidelines, NAMs, 3Rs & Recent Updates in Risk Assessment	Theory + Discussion
2	Day 3	A - Regulatory Toxicology	Testing of Chemicals - Virtual Lab Practical	Practical
2	Day 4	B - AI & Computational Biology	Structural Data Engineering - PDB/mmCIF + PyMOL Visualization	Theory + Practical
3	Day 5	B - AI & Computational Biology	Classical Molecular Docking - AutoDock Vina/AutoDockTools	Practical
3	Day 6	B - AI & Computational Biology	AI-Driven Structure Prediction - AlphaFold3 & ESMFold	Practical
4	Day 7	B - AI & Computational Biology	Generative Docking (DiffDock-L) + ADMET Prediction + Capstone Briefing	Practical
4	Day 8	B - AI & Computational Biology	Network & Systems Biology I - STRING & Cytoscape	Practical
5	Day 9	B - AI & Computational Biology	Network & Systems Biology II - KEGG, DAVID & SwissTargetPrediction	Practical
5	Day 10	C - Research, AI & Biostatistics	AI in Research & Biological Sciences + GraphPad Prism Workshop + Capstone Presentations	Workshop + Presentations
6	Day 11	D - Field Immersion	Forensic Toxicology Visit - AIIMS (Delhi/Faridabad NCR) - Day 1	Field Visit
6	Day 12	D - Field Immersion	Forensic Toxicology Visit - AIIMS (Delhi/Faridabad NCR) - Day 2 + Programme Wrap-up	Field Visit

3. Curriculum

MODULE A - Regulatory Assessment of Toxicology

This module builds the regulatory literacy every toxicologist needs: the rules and frameworks that decide whether a chemical or drug is safe enough to reach the market, and how modern testing is moving away from full reliance on animal studies.

Day	Topic	Sub-topics Covered	Why This Matters
Day 1	OECD Guidelines & Global Regulatory Landscape	OECD Test Guidelines (TG) programme structure Overview of other regulatory bodies: US EPA, ECHA/REACH, CDSO, WHO	Almost all standardised toxicology testing (acute, repeat-dose, genotoxicity, reproductive) is anchored in OECD TGs - this is the common reference language of the field.
Day 2	ICH Guidelines, NAMs, 3Rs & Recent Updates	ICH guidelines (Q, S, M series) relevant to drug safety New Approach Methodologies (NAMs): in vitro, in silico & organ-on-chip approaches The 3Rs principle: Replacement, Reduction, Refinement Recent shifts in toxicology risk assessment (e.g., move toward animal-free safety science)	ICH guidelines govern pharmaceutical safety data internationally; NAMs and the 3Rs represent the direction the entire field is moving toward, and increasingly appear in exams, interviews, and job descriptions.
Day 3	Testing of Chemicals - Virtual Lab Practical	Hands-on session on Vlabs (virtual toxicology/biology laboratories) Simulated acute toxicity / cytotoxicity / enzyme assay experiments Recording and interpreting virtual experiment results in a lab worksheet	Gives practical, procedural exposure to test protocols that would otherwise require wet-lab access - reinforces how theoretical guidelines translate into an actual test.

MODULE B - AI Models in Biology & Toxicology

This is the core computational module. It takes students from retrieving a raw protein structure all the way to running AI-based docking, predicting a molecule's safety/ADMET profile, and mapping its effect across a biological network - the same pipeline used in real computational drug discovery and predictive toxicology labs.

Days 4–6: Structural Data, Classical Docking & AI Structure Prediction

Day	Topic	Tools	Purpose
Day 4	Structural Data Engineering & Visualization	RCSB Protein Data Bank (PDB) & mmCIF Repositories	Primary source for downloading high-resolution macromolecular atomic coordinate files (.pdb/.cif) - the starting point of any structural study.
Day 4	3D Macromolecular Visualization	PyMOL (Schrödinger)	High-resolution 3D rendering, structural alignment, electrostatic surface mapping, and B-factor visualisation of proteins.
Day 5	Classical Computational Docking	AutoDock Vina / AutoDock Tools	Physics-based rigid/semi-flexible receptor-ligand docking, grid-box optimisation, and binding-affinity scoring - the classical benchmark method.
Day 6	AI-Driven Structure Prediction I	AlphaFold 3 Server (Google DeepMind)	Multi-entity structural modelling of complexes with proteins, DNA, RNA, small-molecule ligands, ions, and post-translational modifications.
Day 6	AI-Driven Structure Prediction II	ESMFold (Hugging Face / Meta AI)	Rapid single-chain protein structure prediction directly from sequence, using the ESM-2 protein language model - no MSA required.

Days 7–9: Generative Docking, ADMET & Network Biology

Day	Topic	Tools	Purpose
Day 7	Generative AI Docking	DiffDock-L (Neurosnap AI Server)	Score-based generative diffusion model for unbiased, blind small-molecule docking across an entire protein surface (no predefined binding site needed).
Day 7	ADMET Prediction	ADMETlab 3.0 / SwissADME	Predicts Absorption, Distribution, Metabolism, Excretion and Toxicity properties of a candidate molecule - critical for early safety screening.
Day 7	Capstone Project Briefing	-	Students are assigned/choose one protein target and 2–3 candidate ligands; over the following sessions they will dock, predict ADMET, and map the network effect of their chosen molecule as their mini-project.
Day 8	Protein-Protein Interaction Networks	STRING Database	Construction of physical/functional PPI networks, identification of key signalling hubs, and interaction confidence scoring.
Day 8	Network Visualization & Analysis	Cytoscape	Visual exploration of PPI networks generated in STRING; hub-gene identification using plug-ins such as CytoHubba.

Day 9	Pathway Mapping	KEGG Database	Maps genes/proteins of interest onto known biochemical and signalling pathways to understand mechanism-level context.
Day 9	Functional Annotation & Enrichment	DAVID Functional Annotation System	Gene Ontology (GO) enrichment and clustering, mapping gene sets to biological processes and KEGG pathways.
Day 9	Target Prediction & Off-Target Profiling	SwissTargetPrediction (SIB)	Predicts likely protein targets of a small molecule and flags possible off-target/cross-reactivity - directly relevant to toxicological risk.

4. Software & Platform Checklist

Most tools are free, browser-based servers - only PyMOL and AutoDockTools need local installation. Students should carry a laptop with administrator access and a stable internet connection.

Tool / Platform	Access Type	Used On	Notes
OECD iLibrary / Test Guidelines portal	Free, web	Day 1	Reference guidelines, no login needed
Amrita Vlabs (Virtual Labs)	Free, web	Day 3	Government of India virtual labs initiative
RCSB PDB	Free, web	Day 4	Structure download (.pdb/.cif)
PyMOL (Educational/Open-Source build)	Free install (desktop)	Day 4	Install before Day 4
AutoDock Vina + AutoDockTools (MGLTools)	Free install (desktop)	Day 5	Install before Day 5
AlphaFold 3 Server	Free, web (login)	Day 6	Google account required
ESMFold (Hugging Face Space)	Free, web	Day 6	No login required
DiffDock-L (Neurosnap)	Free/freemium, web	Day 7	Account recommended
ADMETlab 3.0 / SwissADME	Free, web	Day 7	No login required
STRING Database	Free, web	Day 8	No login required
Cytoscape (Desktop)	Free install (desktop)	Day 8	Install before Day 8
KEGG Database	Free, web	Day 9	No login required
DAVID Functional Annotation	Free, web (registration)	Day 9	Register in advance
SwissTargetPrediction	Free, web	Day 9	No login required
GraphPad Prism	Trial/institutional licence	Day 10	Free 30-day trial sufficient; dept. licence preferred
UseGalaxy (RNA-Seq) - optional	Free, web	Self-study	Recommended for further exploration only

MODULE C - Research Skills, AI in Research & Biostatistics

Segment	Topic	Content	Purpose
1 (≈45 min)	AI in Research	How AI tools (literature-summarisation assistants, reference managers, AI writing/analysis aids) are changing the pace of biological & toxicological research	Builds awareness of responsible, efficient use of AI as a research assistant - a skill now expected of every science graduate.
2 (≈45 min)	AI in Biological Sciences - Recap & Bigger Picture	How Days 4–9's tools fit into real pharma/biotech pipelines; career and higher-study relevance	Connects the week's tool-training back to real-world application, motivating further self-learning.
3 (≈90 min)	GraphPad Prism - Statistics Workshop	Data entry & organisation; descriptive statistics; t-test/ANOVA in Prism; generating publication-style graphs; applying this to students' own capstone data	GraphPad Prism is the most widely used statistics/graphing tool in toxicology and pharmacology labs - students leave able to analyse and present their own data.
4 (remaining time)	Capstone Mini-Project Presentations	Each student/group presents their target-ligand docking + ADMET + network-biology mini-project (5–7 min each)	Consolidates the entire computational module into one applied output and gives presentation practice.

MODULE D - Field Immersion: Forensic Toxicology

A 2-day visit to the Department of Forensic Medicine & Toxicology at AIIMS (Delhi/Faridabad NCR region) gives students first-hand exposure to how toxicology is practised in a real medico-legal and clinical setting.

- Orientation to the forensic toxicology laboratory workflow: sample receipt, chain of custody, and case documentation
- Overview of analytical techniques used in post-mortem and clinical toxicology casework (e.g., GC-MS/HPLC-based screening)
- Discussion with resident/faculty toxicologists on real case interpretation and medico-legal reporting
- Reflective field-visit report submitted by each student as part of assessment

5. Mini-Project

Assigned on Day 7 and presented on Last Day, the project is what ties different Modules together into one applied deliverable.

just for an example

- Step 1 - Choose one protein target (e.g., a kinase, receptor, or enzyme relevant to a disease of interest) and retrieve its structure from the PDB, or predict it using AlphaFold3/ESMFold.
- Step 2 - Select 2–3 candidate small molecules and dock them against the target using AutoDock Vina and/or DiffDock-L.
- Step 3 - Run ADMET prediction on the candidate molecules and flag any safety concerns.
- Step 4 - Build a PPI network (STRING/Cytoscape) around the target and map it to a KEGG pathway; run DAVID enrichment if a gene list is available.
- Step 5 - Summarise binding affinities and any group comparisons using GraphPad Prism.
- Step 6 - Present findings in a 5–7 minute talk on Day 10, plus a short written report.

6. Evaluation (4 Credits)

Component	Weightage	Details
Attendance & Participation	10%	Across all 12 contact days
Practical Lab Record	20%	Worksheets/logs from virtual lab (Day 3) and each computational session (Days 4–9)
Module Quizzes / Viva	20%	Short quiz or viva at the end of Module A and Module B
Capstone Mini-Project Report	30%	Written report following the 6-step pipeline in Section 5
Capstone Presentation	15%	5–7 minute presentation on Day 10
Forensic Toxicology Field Report	5%	Reflective report submitted after the AIIMS visit

Certification: A Certificate of Completion (and credit transcript entry) is issued on meeting a minimum 80% attendance threshold and satisfactory completion of the capstone project and field report.

7. Pre-Internship Reading

- OECD Guidelines for the Testing of Chemicals - overview section (oecd.org)
- A short primer on the 3Rs principle (NC3Rs website)
- "What is a protein structure file?" - RCSB PDB's beginner guide
- Any short introductory article/video on AlphaFold and protein structure prediction