Indian Institute of Technology Kanpur

Department of Chemistry

Proposal for a New Course

Course Title	Advances in Chemical Biology and Medicinal Chemistry
Course No.:	CHM6XX
Credits:	3-0-0-0 [9]
Duration of Course:	Full Semester
Proposing Department	Chemistry
Proposing Instructor	Dharmaraja Allimuthu
Offered fo	PG elective
Prerequisite(s) for the course	None
Faculty members interested in teaching	Prof Sandeep Verma and Other Chemical Biology/ Medicinal Chemistry experts
Other Departments/Programmes of whose the students are expected to take up the course	CHM, BSBE, CHE, MSE

Objectives: This PhD-level course equips students with an advanced understanding of medicinal chemistry and chemical biology, emphasizing state-of-the-art drug discovery technologies. Students will explore fundamental and emerging strategies, including structure-based and fragment-based drug design, DNA-encoded libraries, and AI-driven approaches. The course delves into the state-of-the-art drug discovery technologies including covalent therapeutics, proximity inducers (PROTACs, LYTACs, AUTACs, molecular glues & RIPTACs), antibody drug conjugates (ADCs) and RNA-targeted therapeutics, providing a comprehensive view of next-generation drug discovery modalities. Chemical biology techniques such as chemical proteomics, activity-based protein profiling, metabolomics, and lipidomics will be integrated for target identification and mechanism-of-action studies. Computational and biophysical methods, including molecular dynamics, cryo-EM, AI models, and multi-omics, will be applied to accelerate drug discovery. Finally, students will critically evaluate translational challenges, FDA approvals, regulatory considerations, and ethical implications through case studies. By the end of the course, students will be prepared to drive innovations in academia and industry, bridging medicinal chemistry and chemical biology to advance next-generation

therapeutics.

Course Contents

1: Fundamentals and Modern Strategies in Drug Discovery (8 lectures)

- Introduction to Medicinal Chemistry & Chemical Biology – Evolution, key principles, and current challenges
- Chemical Space and Molecular Design – Lipinski's rule, beyond Rule-of-5, and privileged scaffolds
- High-Throughput Screening (HTS) and Fragment-Based Drug Discovery (FBDD)
- Structure-Based and Ligand-Based Drug Design (SBDD, LBDD) – Virtual screening, docking, and scoring functions
- Artificial Intelligence and Machine Learning in Drug Discovery – Deep learning, generative models, and de novo drug design
- Hit-to-Lead Optimization: Medicinal Chemistry Strategies – SAR, ADME, and toxicity considerations
- Emerging Concepts: Click Chemistry and Bioorthogonal Reactions in Drug Development

2: State-of-the-Art Drug Discovery Technologies (8 lectures)

- Proximity inducers: PROTACs, Molecular Glues, LYTACs, AUTACs and RIPTACs. Degrader Design Principles: E3 Ligases, Linker Chemistry, and Protein-Protein Interactions
- Covalent Inhibitors: Mechanisms, Design Strategies and advancements – Warheads, selectivity, and resistance
- mRNA and RNA-Targeted Drug Discovery – Small molecules targeting RNA and RNA-protein interactions
- Antibody-Drug Conjugates (ADCs) and Peptide-Drug Conjugates (PDCs)
- Stapled Peptides, Macrocycles, and Protein-Protein Interaction Inhibitors (PPIIs)
- Next-Generation Therapeutics: CRISPR-Based Gene Editing and Epigenetic Modulators

3: Chemical Biology Approaches in Drug Discovery (8 lectures)

- Multiomics: Metabolomics and Lipidomics in Drug Discovery. Chemical Proteomics for Target Identification – Activity-based protein profiling (ABPP), covalent probes. Photoaffinity Labeling and Chemoproteomics in Target Deconvolution
- Basics of drug-target interactions: Target Engagement and Cellular Thermal Shift Assay

(CETSA), surface plasmon resonance (SPR), isothermal calorimetry (ITC), nuclear magnetic resonance (NMR) spectroscopy .

- Metabolic Labeling and Bioorthogonal Chemistry in Cellular Profiling. Organelle-Targeted Therapeutics – Mitochondria, lysosomes, and autophagy modulators

4: Basics of AI, Computational, and Biophysical Tools for Drug Discovery (8 lectures)

- Computational Approaches: Molecular Docking and Molecular Dynamics Simulations
- AI-Driven Drug Discovery: AlphaFold, DeepMind, and Predictive Modeling. Generative AI for Drug Design: Graph-Based Deep Learning Approaches
- Machine Learning for ADME-Tox Prediction and PK/PD Modeling
- Basics of Cryo-EM, X-ray Crystallography, and NMR for Drug Discovery. Single-Cell and Spatial Proteomics in Drug Mechanism of Action Studies.

5: Case Studies and Translational Strategies (8 lectures)

- Success Stories of First-in-Class Drugs – Lessons from FDA approvals. Clinical Translation of Novel Drug Modalities – PROTACs, ADCs, and mRNA therapeutics.
- Personalized and Precision Medicine: Small Molecule and Biologic Therapeutics
- Industry vs. Academia: Drug Discovery Pipelines and Collaborations. IP, Patents, and Regulatory Challenges in Drug Development
- Ethics in Medicinal Chemistry and Chemical Biology – Dual-use research concerns
- AI-Discovered Drugs in Clinical Trials: Hype vs. Reality. Future Perspectives: Next-Generation Therapeutics and Unmet Challenges

Reference/Textbooks:

1. Essentials of Chemical Biology by Andrew D. Miller (2008/updated)
2. Burger's Medicinal Chemistry, Drug Discovery, and Development (8th ed., 2021)
3. An Introduction to Medicinal Chemistry by Graham L. Patrick (6th ed., 2017)
4. The Practice of Medicinal Chemistry by Camille G. Wermuth (5th ed., 2015)
5. Antibody-Drug Conjugates: Fundamentals, Drug Development, and Clinical Outcomes (Wiley, 2017/updated)
6. Multi-Omics Technology in Human Health and Diseases (Elsevier, 2025) by Macha et al
7. Molecular Docking for Computer-Aided Drug Design by S. G. Coumar (Academic Press, 2021)
8. Artificial Intelligence in Drug Discovery (RSC, 2020/updated)

9. Latest Research papers will be discussed

Course Proposed by	Forwarded by	Course is Approved/ Not approved
Dharmaraja Allimuthu	Convenor, DPGC	Chairperson, SPGC