



MEDICINAL CHEMISTRY

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PRE-REQUISITES : Any student who has done basic organic chemistry and has some knowledge of biochemistry with an interest in drug discovery

INTENDED AUDIENCE : Third year undergraduates of B.Sc. Chemistry; M.Sc. Chemistry students and doctoral students

INDUSTRIES APPLICABLE TO : Companies in the pharmaceutical sector may recognize and value this course.

COURSE OUTLINE :

The main objective of this course is to familiarize students with the fundamental concepts of drug discovery and development. The course is intended for students who have a background in chemistry and interested in the process of drug discovery. The intended outcome is to train students on various aspects of new drug discovery/development, drug screening, target identification, lead discovery, optimization and the molecular basis of drug design and drug action.

ABOUT INSTRUCTOR :

Prof. Harinath Chakrapani completed his undergraduate and post-graduate studies in Chemistry from Loyola College and Indian Institute of Technology Madras, respectively. He moved to Duke University, USA to pursue his doctoral studies and after post-doctoral research stints at Wake Forest University and the National Cancer Institute, USA, he joined IISER Pune in July 2009 and is currently Associate Professor.

COURSE PLAN :

Week 1: An overview of drugs and drug targets; structure of a cell; intermolecular binding forces; classification of drugs.

Week 2: Principles of enzyme structure, catalysis and inhibition in drug discovery: enzyme catalysis and inhibition in drug discovery;

Week 3: Principles of enzyme structure, catalysis and inhibition in drug discovery: Enzyme mechanisms overview; case

Week 4: Receptors function and ligand binding interactions; Ion channel receptors; kinase-linked receptors; G-Protein coupled receptors, drug-receptor interaction; dose-response curves; case

Week 5: Nucleic acids structure and function; DNA Interactive agents and chemotherapy: DNA binding agents; intercalation and alkylation; DNA strand breakers; case studies

Week 6: Synthetic methods in medicinal chemistry: Combinatorial and parallel synthesis: solid phase techniques, mix and split method in combinatorial synthesis;

Week 7: Lead discovery; Bioassays; drug targets; Lead Modification; optimization; pharmacophore; homologation; bioisostere; chain branching;

Week 8: Electronic effects; Lipophilicity; Structure-Activity Relationships; Quantitative-structure activity relationships (QSAR).

Week 9: Drug metabolism and pharmacology: Analytical methods in metabolism; Phase I and II transformations; ADME; bioavailability; pre-clinical and clinical development; therapeutic index and therapeutic window.

Week 10: Prodrugs and drug delivery systems: Use of prodrug systems; prodrugs for stability, solubility and slow release; overview of drug delivery

Week 11: Drug resistance mechanisms and synergism: Mechanisms of drug resistance;

Week 12: circumventing drug resistance; drug synergy