MEDICINAL CHEMISTRY

CHEMISTRY AND BIOCHEMISTRY

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IISER Pune

TYPE OF COURSE : New | Core| UG/PG

COURSE DURATION : 12 weeks (28 Jan'19 - 19 Apr'19)

EXAM DATE : 27 Apr 2019

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

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 :

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. His research interests are in organic chemistry and chemical biology. His laboratory works on developing new tools to study effects of oxidative stress responses in cells and antibiotic resistance. He has over eight years of teaching experience at IISER Pune.

COURSE PLAN :

Week 01 : An overview of drugs and drug targets; structure of a cell; intermolecular binding forces; classification of drugs.

Week 02 : Principles of enzyme structure, catalysis and inhibition in drug discovery: Enzyme mechanisms overview; enzyme catalysis and inhibition in drug discovery; reversible and irreversible inhibitors; transition-state inhibitors; case studies

Week 03 : Principles of enzyme structure, catalysis and inhibition in drug discovery: Enzyme mechanisms overview; enzyme catalysis and inhibition in drug discovery; reversible and irreversible inhibitors; transition-state inhibitors; case studies,Receptors function and ligand binding interactions; Ion channel receptors; kinase-linked receptors; G-Protein coupled receptors, drug-receptor interaction; dose-response curves; case studies

Week 04 : Receptors function and ligand binding interactions; Ion channel receptors; kinase-linked receptors; G-Protein coupled receptors, drug-receptor interaction; dose-response curves; case studies

Week 05 : Nucleic acids structure and function; DNA Interactive agents and chemotherapy: DNA binding agents; intercalation and alkylation; DNA strand breakers; case studies

Week 06 : Synthetic methods in medicinal chemistry: Combinatorial and parallel synthesis: solid phase techniques, mix and split method in combinatorial synthesis; dynamic combinatorial synthesis; solid phase synthesis; diversity-oriented synthesis.

Week 07 : Lead discovery; Bioassays; drug targets; Lead Modification; optimization; pharmacophore; homologation; bioisostere; chain branching; Electronic effects; Lipophilicity; Structure-Activity Relationships; Quantiative-structure activity relationships (QSAR).

Week 08 : Lead discovery; Bioassays; drug targets; Lead Modification; optimization; pharmacophore; homologation; bioisostere; chain branching; Electronic effects; Lipophilicity; Structure-Activity Relationships; Quantiative-structure activity relationships (QSAR).

Week 09 : Drug metabolism and pharmacology: Analytical methods in metabolism; Phase I and Phase II transformations; Absorption, distribution, metabolism and excretion (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 - 12 : Drug resistance mechanisms and synergism: Mechanisms of drug resistance; circumventing drug resistance; drug synergy