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| Semester | JAN 2022 |
| Open to semester | 8,14,22 |
| Course code | **CHM423/CH6264** |
| Course title | **Medicinal Chemistry** |
| Credits | 4 /4 |
| Course Coordinator & participating faculty (if any) | Raghavendra Kikkeri |
| Nature of Course | Lectures |
| Pre-requisites | Any Student with organic chemistry with basic biology background |
| Objectives (goals, type of students for whom useful, outcome etc) | 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 biology interested in the process of drug discovery |
| Course contents (details of topics /sections with no. of lectures for each) | Drug discovery overview; discovery without a lead; Lead discovery; pre-clinical development and clinical trials etc.<br>• Receptors function and ligand binding interactions; theories of drug-receptor interaction; dose-response curves<br>• Principles of enzyme structure, catalysis and inhibition in drug discovery: Enzyme mechanisms overview; enzyme catalysis and inhibition; reversible and irreversible inhibitors<br>• DNA Interactive agents and chemotherapy: DNA binding agents; intercalation and alkylation; DNA strand breakers<br>• Drug Targets: Receptors, enzymes, nucleic acids, miscellaneous targets<br>• Drug metabolism and pharmacology: Absorption, distribution, metabolism and excretion (ADME); Phase I and Phase II transformations; therapeutic index; bioavailability etc.<br>• Lead Modification, Structure-Activity Relationships; Optimization of drug-target interactions; pharmacophore identification; extension and rigidification tactics; homologation; chain branching; optimizing access to the target<br>• Quantitative-Structure-Activity Relationship (QSAR): Lipophilicity; measures of sterics; bioisosteres etc.<br>• Synthetic methods in medicinal chemistry: Combinatorial |

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| | and parallel synthesis: solid phase techniques, mix and split method in combinatorial synthesis; dynamic combinatorial synthesis; solid phase synthesis; diversity-oriented synthesis.<br>• Computational methods in drug discovery: An overview of computational methods; 3D pharmacophore identification; virtual screening; basics of docking<br>• Case Studies: Anti-bacterial drugs; anti-cancer drugs; anti-viral drugs; drugs acting on the nervous system; anti-ulcer compounds.<br>• Drug resistance mechanisms and synergism: Mechanisms of drug resistance; circumventing drug resistance; drug synergy<br>• Prodrugs and drug delivery systems: Use of prodrug systems; carrier-linked prodrugs; prodrugs for stability, solubility and slow release; Bioprecursor prodrugs; macromolecular delivery systems.<br>• Advanced topics: Strategies towards target Identification; screening |
| Evaluation /assessment | End-Sem Examination-35%<br>Mid-Sem Examination-50%<br>Others-15% Assignment and presentation% |
| Suggested readings (with full list of authors, publisher, year, edn etc.) | An Introduction to Medicinal Chemistry, Graham L. Patrick; Second Edition (Primary)<br>The Organic Chemistry of Drug Design and Drug Action, Richard B. Silverman, Second Edition |