BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

INSTRUCTION DIVISION

Semester I; 2015-16
Course Handout Part II

Date: 03-8-2015

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further details regarding the course.

Course No:	**CHEM F335**
Course Title:	**Organic Chemistry and Drug Design**
Instructor-in-charge:	Paritosh Shukla
Instructor:	Paritosh Shukla

1. **Scope and objective of the course:** To familiarize the students with basic aspects of drug discovery and more importantly, the applications of organic chemistry in drug design, important drug targets, marketed drugs, synthesis of drugs; the overall objective is to have a reflective teaching and learning environment

2. Text Book (T1): An Introduction to Medicinal Chemistry by Graham L. Patrick, Oxford University Press, 3'rd Ed.
Reference Books (R1): T. Morrison and R. Boyd, Organic Chemistry, Pearson, 7th ed., 2011

3. Learning Outcomes: The learner should be able to accomplish the following:

- Able to identify and list at least five biological targets for drugs
- From the above targets, be able to analyze and choose suitable targets for a disease with rationale
- For the above targets be able to identify ten important available drugs, with the corresponding Structure-Activity Relationship (SAR)
- Singly or in groups, be able to use Autodock software to dock a drug to the target of his choice
- At the end, be able to rationally design and propose simple synthesis of a drug for a disease of his choice.

4. Course Plan:

Lec. No.	Learning objectives	Topics to be Covered	Text book (topic no.)
1-5	Introduction to biomolecules	a) Lipids: Fats, Steroids, Terpenes, prostaglandins b) Alkaloids c) Amino acids and proteins d) Enzymes, Co-enzymes and Vitamins e) Nucleic acids: nucleotides and nucleosides	R1: Ch. 25; 27-30
6	Drug targets	Basic idea of why, how, and where drugs work; idea of drug targets	Ch.1

7-8	Proteins as drug targets	structure of proteins; peptides as drugs; enzyme inhibitors; enzyme kinetics; Receptor role and action; affinity, efficacy, and potency;	Ch. 3,4,5
9-10	Nucleic acids as drug targets	Structure of DNA and RNA; genetic illness, molecular biology and genetic engineering	Ch. 7
11-12	Pharmacokinetics (PK)	Basic PK; its applications to drug discovery; elementary idea of ADMET properties	Ch. 8
13-16	Drug discovery, design, and development	a) finding a lead; choosing a disease, target, and bioassay; finding leads from natural drugs, libraries, existing drugs b) optimizing target interactions; SAR c) drug development: preclinical and clinical trials; patenting	Corresponding Ch in T1
17-20	Latest tools	QSAR; combinatorial synthesis; x-ray; docking	Corresponding Ch in T1
21-25	Antibacterial agents	Sulfonamides; penicillins; cephalosporins; β-lactam antibiotics: introduction, synthesis, and design	Corresponding Ch in T1
26-30	Antiviral agents	Against DNA viruses; against RNA viruses/HIV; protease inhibitors: introduction; synthesis, and design	Corresponding Ch in T1
31-34	Anticancer agents	Cancer; drugs acting on nucleic acids; antimetabolites; hormone-based therapies; inhibitors of signaling pathways	Corresponding Ch in T1
35-40	Other drugs	Cholinergics; andrenergic nervous system (β-blockers); opiates (opium, morphine, analgesics); antiulcer drugs	Corresponding Ch in T1

Evaluation components:

Component	Duration	Weightage (%)	Remarks	Date and Time
Mid-semester Test	90 min	30	CB[2]	5/10 2:00 - 3:30 PM
Tutorial tests + Seminar + Group activity	10 min each	30	Continuous	
Comprehensive Examination	3 hrs	40	OB[3] + CB	2/12 FN

[1]TBA: To Be Announced; [2]CB: Closed Book; [3]OB: Open Book.

5. Make-up(s) will be granted only for genuine reasons decided by the instructor.

6. Notices: All the notices pertaining to this course will be displayed on **Chemistry Dept. Notice Board only**.

Instructor-in-Charge