

INSTITUTE	FACULTY OF PHARMACY
PROGRAM	MASTER OF PHARMACY (PHARMACEUTICS)
SEMESTER	2
COURSE TITLE	COMPUTER-AIDED DRUG DEVELOPMENT
COURSE CODE	13MC0203
COURSE CREDITS	4

Objective:

- 1 This course is designed to impart knowledge and skills necessary for computer Applications in pharmaceutical research and development who want to understand the application of computers across the entire drug research and development process. Basic theoretical discussions of the principles of more integrated and coherent use of computerized information (informatics) in the drug development process is provided to help the students to clarify the concepts.
- 2 This course is designed to impart knowledge and skills necessary for computer Applications in pharmaceutical research and development who want to understand the application of computers across the entire drug research and development process. Basic theoretical discussions of the principles of more integrated and coherent use of computerized information (informatics) in the drug development process is provided to help the students to clarify the concepts.

Course Outcomes: After completion of this course, student will be able to:

- 1 Understand computational modeling in drug disposition and optimization techniques in pharmaceutical formulation
- 2 Understand computer simulation in pharmacokinetics, pharmacodynamics, biopharmaceutical characterization, and clinical development
- 3 Understand Artificial Intelligence (AI), robotics and computational fluid dynamics(CFD)

Pre-requisite of course:Nil

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
4	0	0	75	15	10	0	0

Contents : Unit	Topics	Contact Hours
1	Unit-1 a. Computers in Pharmaceutical Research and Development: A General Overview: History of Computers in Pharmaceutical Research and Development. Statistical modeling in Pharmaceutical research and development: Descriptive versus Mechanistic Modeling, Statistical Parameters, Estimation, Confidence Regions, Nonlinearity at the Optimum, Sensitivity Analysis, Optimal Design, Population Modeling, b. Quality-by-Design In Pharmaceutical Development: Introduction, ICH Q8 guideline, Regulatory and industry views on QbD, Scientifically based QbD - examples of application.	12
2	Unit-2 Computational Modeling Of Drug Disposition: Introduction, Modeling Techniques: Drug Absorption, Solubility, Intestinal Permeation, Drug Distribution, Drug Excretion, Active Transport; P-GP, BCRP, Nucleoside Transporters, hPEPT1, ASBT, OCT, OATP, BBB-Choline Transporter.	12
3	Unit-3 Computer-aided formulation development: Concept of optimization, Optimization parameters, Factorial design, Optimization technology & Screening design., Computers in Pharmaceutical Formulation: Development of pharmaceutical emulsions, microemulsion drug carriers Legal Protection of Innovative Uses of Computers in R&D, The Ethics of Computing in Pharmaceutical Research, Computers in Market analysis	12
4	Unit-4 a. Computer-aided biopharmaceutical characterization: Gastrointestinal absorption simulation. Introduction, Theoretical Background, Model construction, Parameter sensitivity analysis, Virtual trial, Fed vs. fasted state, In vitro dissolution and in vitro in vivo correlation, Biowaiver considerations, b. Computer Simulations in Pharmacokinetics and Pharmacodynamics: Introduction, Computer Simulation: Whole Organism, Isolated Tissues, Organs, Cell, Proteins, and Genes., c. Computers in Clinical Development: Clinical Data Collection and Management, Regulation of Computer Systems	12
5	Unit-5 Artificial Intelligence (AI), Robotics and Computational fluid dynamics: General overview, Pharmaceutical Automation, Pharmaceutical applications, Advantages, and Disadvantages. Current Challenges and Future Directions.	12
Total Hours		60

Textbook :

- 1 Computer Applications in Pharmaceutical Research and Development, Sean Ekins, John Wiley & Sons., 2006

Textbook :

- 2 Computer-Aided Applications in Pharmaceutical Technology, Jelena Djuris, Woodhead Publishing, 2003
- 3 Encyclopedia of Pharmaceutical Technology, James Swarbrick, James. G.Boylan, Marcel Dekker Inc, New York, 1996

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery					
Remember / Knowledge	Understand	Apply	Analyze	Evaluate	Higher order Thinking / Creative
20.00	25.00	25.00	15.00	15.00	10.00

Instructional Method:

- 1 The course delivery method will depend upon the requirement of content and the need of students. The teacher in addition to the conventional teaching method by the blackboard may also use any tools such as demonstration, role play, quiz, brainstorming, MOOCs etc.
- 2 The internal evaluation will be done based on continuous evaluation of students in the laboratory and classroom.
- 3 Students will use supplementary resources such as online videos, NPTEL videos, MOOCs/ e-courses, virtual laboratories.