GUJARAT TECHNOLOGICAL UNIVERSITY

M.Pharm

Pharmaceutics (20)

SEMESTER: II

Subject Name: COMPUTER AIDED DRUG DEVELOPMENT
Subject Code: MPH203T

Scope: This course is designed to impart knowledge andskills 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 are provided to help the students to clarify the concepts.

Objectives: Upon completion of the course student shall be able to understand

1. History of Computers in Pharmaceutical Research and Development
2. Computational Modeling of Drug Disposition
3. Computers in Preclinical Development
4. Optimization Techniques in Pharmaceutical Formulation
5. Computers in Market Analysis
6. Computers in Clinical Development
7. Artificial Intelligence(AI) and Robotics
8. Computational fluiddynamics (CFD)

Sr.	Topic	Hr
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 Q8guideline, Regulatory and industry views on QbD, Scientifically based QbD-examples of application	**12**
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-CholineTransporter	**12**
3.	Computer-aided formulation development:: Concept of optimization, Optimization parameters, Factorial design, Optimization technology & Screening design. Computers in Pharmaceutical Formulation: Development of pharmaceutical emulsions, micro emulsion 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.	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 vitroin 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.	Artificial Intelligence (AI), Robotics and Computational fluid dynamics: General overview, Pharmaceutical Automation, Pharmaceutical applications, Advantages and Disadvantages. Current Challenges and Future Directions	**12**

REFERENCES:

1. Computer Applications in Pharmaceutical Research and Development, Sean Ekins,2006,JohnWiley&Sons.
2. Computer-Aided Applications in Pharmaceutical Technology, 1st Edition, JelenaDjuris,Woodhead Publishing 3. Encyclopedia of Pharmaceutical Technology, Vol 1
3. James Swarbrick, James.G.Boylan,MarcelDekkerInc,New York,1996**.**