



Shree H. N. Shukla Institute of Pharmaceutical Education & Research

(Affiliated to Gujarat Technological University, Approved by PCI)

Shree H. N. Shukla College Campus, Nr. Lalpari Lake, B/H. Marketing Yard,
Amargadh – Bhichari, Raikot. Mo. 9099063150, 9727753360

M.Pharm Pharmaceutics (20) SEMESTER: II

Subject Name: COMPUTER AIDED DRUG DEVELOPMENT

Subject Code: MPH203T

Scope: 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 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 fluid dynamics (CFD)

Teaching scheme and examination scheme:

Teaching Scheme				Evaluation Scheme			
Theory	Tutorial	Practical	Total	Theory		Practical	
				External	Internal	External	Internal
4	0	0	4	80	20	0	0

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 Q8 guideline, 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-Choline Transporter	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 vitro	12



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	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	
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, John Wiley & Sons.
2. Computer-Aided Applications in Pharmaceutical Technology, 1st Edition, Jelena Djuris, Woodhead Publishing
3. Encyclopedia of Pharmaceutical Technology, Vol 1
3. James Swarbrick, James.G.Boylan, Marcel Dekker Inc, New York, 1996.

LEARNING OUTCOMES:

UNIT	LEARNING OUTCOME
1	Knowledge regarding the Computers in Pharmaceutical Research and Development.
2	Understand the Computational Modeling Of Drug Disposition.
3	Appreciate the Computational Modeling Of Drug Disposition
4	Knowledge Computer-aided biopharmaceutical characterization.
5	Understand the Computer-aided biopharmaceutical characterization.

BOOK LIST:

Sr. no	Book name	Price (Rs.)
1	Computer Applications in Pharmaceutical Research and Development, Sean Ekins, 2006, John Wiley & Sons.	9,867/-
2	Computer-Aided Applications in Pharmaceutical Technology, 1st Edition, Jelena Djuris, Woodhead Publishing	8,950/-
3	Encyclopedia of Pharmaceutical Technology, Vol 1.	
3	James Swarbrick, James.G.Boylan, Marcel Dekker Inc, New York, 1996.	1,58,553/-