



Faculty of Pharmacy
Master of Pharmacy (M. Pharm.)
(W. E. F.: 2023-24)
Document ID: SUTEFPHM-01

Name of Faculty	:	Faculty of Pharmacy
Name of Program	:	Master of Pharmacy (M. Pharm)
Course Code	:	2MPH03
Course Title	:	Computer Aided Drug Development
Type of Course	:	Pharmaceutics
Year of Introduction	:	2023-24

Prerequisite	:	To have sufficient knowledge about basics of pharmaceutical dosage forms
Course Objective	:	This course will discuss the following aspects of <ol style="list-style-type: none"> 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 Robot 8. Computational fluid dynamics (CFD)
Course Outcomes	:	Upon successful completion of this course, the students will be able to
	CO1	To learn about basics of computer and its implementation in R & D in pharmaceutical industry.
	CO2	To learn about various computerized models for its use in pharma industry.
	CO3	To understand about usage of computer in formulation and evaluation for various dosage forms.
	CO4	To understand about AI (Artificial Intelligence) and its usage in pharmaceutical industry.

Teaching and Examination Scheme

Teaching Scheme (Contact Hours)			Credits	Examination Marks				
				Theory Marks		Practical Marks		Total Marks
L	T	P	C	SEE	CIA	SEE	CIA	
04	00	00	04	75	25	00	00	100

Legends: L-Lecture; T-Tutorial/Teacher Guided Theory Practice; P - Practical, C - Credit, SEE - Semester End Examination, CIA - Continuous Internal Assessment (It consists of Assignments/Seminars/Presentations/MCQ Tests, etc.)

Course Content

Unit No.	Topics	Teaching Hours	Weightage	Mapping With COs
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	20%	CO1
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	20%	CO2
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	20%	CO3
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	12	20%	CO1, CO2

	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	20%	CO4

Suggested Distribution of Theory Marks Using Bloom's Taxonomy						
Level	Remembrance	Understanding	Application	Analyse	Evaluate	Create
Weightage	50	50	-	-	-	-

NOTE: This specification table shall be treated as a general guideline for the students and the teachers. The actual distribution of marks in the question paper may vary slightly from above table.

Suggested Learning Websites

Sr. No.	Name of Website
1	https://pci.nic.in/pdf/Syllabus_B_Pharm.pdf
2	https://www.aicte-india.org/downloads/bpharma.pdf
3	https://www.ipc.gov.in/
4	https://www.ayush.gov.in/
5	https://ayudmla.gujarat.gov.in/home.php
6	https://www.fda.gov/
7	https://www.pharmacopoeia.com/
8	https://ipapharma.org/
9	https://gpat.nta.nic.in/
10	https://drnaitiktrivedi.com/
11	https://gdc4gpat.com/course/gpat/
12	https://niscpr.res.in/
13	https://delnet.in/
14	https://ihubgujarat.in/
15	https://www.ssipgujarat.in/



Reference Books

Sr. No.	Name of Reference Books
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 13, James Swarbrick, James. G.Boylan, Marcel Dekker Inc, New York, 1996.