

# LJ UNIVERSITY

LJ INSTITUTE OF PHARMACY

Department of Pharmaceutical Technology

SEMESTER III

**Subject Name: COMPUTER AIDED DRUG DELIVERY SYSTEM**

**Subject Code: MPH301T**

**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, it is expected that the students will be able to:

1. Understand the history of computers in pharmaceutical research and requirements of quality by design in pharmaceutical development.
2. Identify the computational modelling of drug disposition.
3. Select the computer-aided optimization techniques in pharmaceutical formulation.
4. Utilize the computer in Pre-clinical and Clinical development.
5. Apply the concept of Artificial Intelligence, Robotics and Computational fluid dynamics.

**Teaching scheme and examination scheme:**

Teaching Scheme				Evaluation Scheme	
Theory	Tutorial	Practical	Total	Theory	
				External	Internal
4	0	0	4	75	25

Sr. No.	Course Contents	Hours
1	A.) <b>Computers in Pharmaceutical Research and Development:</b> A General Overview: History of Computers in Pharmaceutical Research and Development. Statistical modelling in pharmaceutical research and development: Descriptive versus Mechanistic Modelling, Statistical Parameters, Estimation, Confidence Regions, Nonlinearity at the Optimum, Sensitivity Analysis, Optimal Design, Population Modelling.  B.) <b>Quality-by-Design in Pharmaceutical Development:</b> Introduction, ICH Q8 guideline, Regulatory and industry views on QbD, scientifically based QbD - examples of application.	12
2	<b>Computational Modelling of Drug Disposition:</b> Introduction ,Modelling Techniques: Drug Absorption, Solubility, Intestinal Permeation, Drug Distribution ,Drug Excretion,	12

	Active Transport; P-gp, BCRP, Nucleoside Transporters, hPEPT1, ASBT, OCT, OATP, BBB-Choline Transporter.	
3	<b>Computer-aided formulation development:</b> 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	A.) <b>Computer-aided biopharmaceutical characterization:</b> 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.) <b>Computer Simulations in Pharmacokinetics and Pharmacodynamics:</b> 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	<b>Artificial Intelligence (AI), Robotics and Computational fluid dynamics:</b> General overview, Pharmaceutical Automation, Pharmaceutical applications, Advantages and Disadvantages. Current Challenges and Future Directions.	12
<b>Total Hours</b>		<b>60</b>

#### Recommended 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.