

# COURSE MODULE

Program Title	M. Pharmacy Pharmacology Principle of Drug Discovery			
Department				
Course Title				
1. NAME OF INSTITUTION	: Y. B. CHAVAN COLLEGE OF PHARMACY, AURANGABAD			
2. AFFILIATED UNIVERSITY	: DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD			

3.	DEPARTMENT	:	PHARMACOLOGY
4.	PROGRAM TITLE	:	M. PHARM.

4.1. Program Specific Outcome:

After completing the program, the student will be able to:

M. Pharm in Pharmacology: After completion of the program, the student will be able to:

**PSO 01:** Highlight advancement in knowledge associated with advance pharmacology, toxicology, molecular pharmacology, drug discovery, clinical research and pharmacovigilance.

**PSO 02:** Independently carry out research and development work in pharmacology and interdisciplinary areas utilizing modern tools and employing problem analysis skills to solve practical problems.

PSO 03: Build the professional skills, computational, analytical and critical thinking skills.

**PSO 04:** Build protocols to test efficacy, safety and toxicity of the new chemical entities as per the guidelines.

PSO 05: Apply the GLP concepts, CCSEA and OECD guidelines in animal studies.

## 5. COURSE SPECIFICATION :

#### **5.1.**Course Identification and General Information

a. Course Title:	PRINCIPLES OF DRUG DISCOVERY		
b. Course Number/Code	MPL 203T		
c. Credit Hours	Theory	Practical	
	04	NA	
d. Study level/semester at which this	Sem II		
course is offered			
e. Pre-requisite	B. Pharm Pharmaco	logy III	
f. Co-requisite	Pharmacodynamics, Pharmacokinetics, Drug		
	discovery, Targets of drug discovery.		
g. Program in which the course is offered	M Pharm		
h. Language of teaching the course	English		
i. Prepared by	Mr. Mohd Mukhtar	khan	
	Dr. Nikhil Sakle		
j. Approved by HOD	Dr. Syed Ayaz Ali		

## **5.2.Course Description:**

The subject imparts a fundamental knowledge role of genomics, proteomics and bioinformatics in drug discovery process. This information will further help the student to apply the knowledge in computer aided drug design in drug discovery.

## **5.3.Course Objectives:**

- Explain the various stages of drug discovery processes.
- Explain the molecular pathways related to Genomics and proteomics
- Appreciate the applicability of computer aided drug design in drug discovery process.
- Demonstrate molecular biology techniques as applicable for pharmacology.

### 6.0.Course Outcomes (COs) : (Min. 4 and Max. 6)

### (Use Bloom's Taxonomy words)

CO Code	Course outcome			
CO-104.1	To provide students with an understanding of the process of drug discovery and development from the identification of novel drug targets			
CO-104.2	Demonstrate and find new drugs into clinical practice.			
CO-104.3	Relate with principles and applications of genomic and proteomic tools.			
CO-104.4	Explain detailed concepts of computer aided drug design in drug discovery process.			
CO-104.5	Elaborate the techniques in computer aided drug design in drug discovery.			

## 6.1. Knowledge and Understanding

### (Alignment of PSOs to COs)

Course Code	Program Specific			
	Outcome			
	PSO-1	PSO-2	PSO-3	PSO-4
CO-104.1	3	1	1	1
CO-104.2	3	-	2	-
CO-104.3	2	2	3	1
CO-104.4	1	2	3	-
CO-104.5	3	3	3	-

Correlation levels 1, 2 or 3 as defined below:

1: Slight (Low); 2: Moderate (Medium);

3: Substantial (High); If there is no correlation, put '-'

## 6.2. Teaching and Assessment Methods for achieving learning outcome:

Teaching Strategies(methods)/Tools used	Methods of Assessment
Lectures (Constructivist learning)	Formative Assessment
Collaborative learning (Discussion)	Case study
Project based Learning	Class test
Blended learning	Multiple choice questions
Inquiry based learning	Assignments
Flash cards	Seminar
Video	Viva Voce
Equipment models	Synopsis
	Tutorials
	Summative Assessment

## **6.3.**Tools for the Teaching and learning

Theory subjects	Practical Subjects
PowerPoints presentation	White boards
• Videos	• Glassware
Flash Card	Chemicals
• Models	• Instruments
Software	• Equipment
• Charts	Software
Smart Boards	• Models
White boards	Plants/Crude Drugs
Online Platform	• Animal

## **6.4.COURSE CONTENT**

**6.1. Theoretical Aspect:** 

Order Topic list/units		Subtopics list	Number	Contact
			of	Hours
			Weeks	
1	Unit I	An overview of modern drug discovery process:	03	12
		Identification, target validation, lead identification and lead Hrs Optimization, Economics of drug discovery. Target Discovery and validation-Role of Genomics, Proteomics and Bioinformatics. Role of Nucleic acid microarrays, Protein microarrays, Antisense technologies, siRNAs, antisense oligonucleotides, Zinc finger proteins. Role of transgenic animals in target validation.		
2	Unit II	Lead Identification-	03	12
		combinatorial chemistry & high throughput screening, in silico lead discovery techniques, Assay development For hit identification. Protein structure Levels of protein structure, Domains, motifs, and folds in protein Structure. Computational prediction of protein structure: Threading and homology modelling methods. Application of NMR and X-ray crystallography in protein structure prediction		
3	Unit III	Rational Drug Design Traditional vs rational drug design, Methods followed in traditional drug design. High throughput screening. Concepts of Rational Drug Design, Rational Drug Design Methods: Structure and Pharmacophore based approaches Virtual Screening techniques: Drug likeness screening, Concept of pharmacophore mapping and pharmacophore based Screening.	03	12
4	Unit IV	Molecular docking: Rigid docking, flexible docking, manual docking; Docking based screening. De novo drug design. Quantitative analysis of Structure Activity Relationship History and development of QSAR, SAR versus QSAR, Physicochemical parameters, Hansch analysis, Fee Wilson analysis and relationship between them.	03	12
5	Unit V	QSAR Statistical methods regression analysis, partial least square analysis (PLS) and other multivariate statistical methods. 3D-QSAR approaches like COMFA and COMSIA Prodrug design-Basic concept, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action. Rationale of prodrug design and practical consideration of prodrug design.	03	12
	TOTAL		15	60

Order	Name of Experiment	Number of Weeks
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		

## 6.2.Practical Aspects - NA

## 7.0. ASSESSMENT MECHANISM:

Sr.	Assessment Mechanism	Week due	Marks	Proportion of Final
No.				Assessment
1	Continuous Assessment (Theory)	2 <sup>nd</sup> week of every month	10	4%
2	Sessional (Internal Theory exam)	As per schedule of examination	15	6%
3	Continuous Practical Assessment (Sessional Practical exam)	Weekly during practical	20	8%
4	Sessional (Internal Practical exam)	As per schedule of examination	30	12%
5	Final exam (theory)	As per University at end of course	75	30%
6	Final exam(practical)		100	40%
Total			150	100%

## **8.0.STUDENT SUPPORT:**

Office hours/week	Other procedures
Two hours minimum	Mr. Mukhtar Khan <u>mukhtarpharma@gmail.com</u> Dr. Nikhil Sakle <u>nikhilsakle@gmail.com</u>

## 9.0.TEACHER'S AVAILABILITY FOR STUDENT SUPPORT:

Days	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
Time	12:00-1:00	12:00-1:00	12:00-1:00	12:00-1:00	12:00-1:00	12:00-1:00

### **10.0. LEARNING RESOURCES:**

Sr.No.	Title of Learning Material	Details
1	Text books	1. MouldySioud. Target Discovery and Validation
		Reviews and Protocols: Volume 2 Emerging
		Molecular Targetsand Treatment Options. 2007
		Humana Press Inc.
		2. Darryl León. Scott Markelin. Silico Technologies in
		Drug Target
		Identification and Validation. 2006 by Taylor and
		Francis Group, LLC.
		3. Johanna K. DiStefano. Disease Gene Identification.
		Methods and
		Protocols. Springer New York Dordrecht Heidelberg
		London. 4. Hugo Kubiny. QSAR: Hansch Analysis and
		Related Approaches. Methods and Principles in
		Medicinal Chemistry, Publisher Wiley-VCH
		5. Klaus Gubernator, Hans-Joachim Böhm. Structure-
		Based Ligand Design.
		Methods and Principles in Medicinal Chemistry.
		Publisher Wiley-VCH 6. Abby L. Parrill. M Rami
		Reddy. Rational Drug Design. Novel Methodology and
		Practical Applications. ACS Symposium Series:
		American Chemical Society: Washington, DC, 1999.
2	Reference material	Text books in college library
3	E-materials and websites	You tube videos, e-books, slide share
4	Other learning material	

## **11.0. FACILITIES REQUIRED:**

Sr.No.	Particular of Facility Required
1	Lecture Rooms (capacity for 60 students)
2	Laboratory (capacity for 20 students)
3	Computing resources: PC with latest version and hardware/software and utilization of open source and licensed application software
4	Other resources: Appropriate laboratory tools, Chemicals, Glass ware, Apparatus, Instrumentation

## 12.0. COURSE IMPROVEMENT PROCESSES:

### 12.1. Strategies for obtaining student feedback on effectiveness of teaching:

Course delivery evaluation by students using: Questionnaire forms and online questionnaires

## 12.2. Other strategies for evaluation of teaching by the instructor or by the department:

Periodic review by Academic Planning & Monitoring Committee and departmental review committee, Observations and assistance of colleagues, External assessments by advisors/ examiners and auditors.

### **12.3.** Process for improvement of teaching:

Use of ICT tools, teaching aids, Simultaneous practical orientation and theory classes (SPOT), Adoption of reflective teaching.

## **12.4.** Describe the planning procedures for periodically reviewing of course effectiveness and planning for improvement:

Periodic review by departmental meeting, Review of course delivery and outcome through assessment and feedback from all stake holders.

### 12.5. Course development plans:

Provide inputs for course improvement and update to University Course development Committees (Board of Studies)

## 13.0. INFORMATION ABOUT FACULTY MEMBER RESPONSIBLE FOR THE COURSE:

Name	Mr. Mohd Mukhtar khan
Location	Department of Pharmacology
Contact Detail (e-mail &cell no.)	9960833118(mukhtarpharma@gmail.com)
Office Hours	10:00 AM to 5:00 PM

Name	Dr. Nikhil Sakle (NSS)
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