COURSE MODULE

Program Title	M. Pharmacy
Department	Pharmaceutical Chemistry
Course Title	Computer Aided Drug Design (MPC 203T)

1. **NAME OF INSTITUTION** : Y. B. Chavan College Of Pharmacy, Aurangabad

2. **AFFILIATED UNIVERSITY** : Dr. Babasaheb Ambedkar Marathwada University, Aurangabad

3. **DEPARTMENT** : Pharmaceutical Chemistry

4. **PROGRAM TITLE** : M. Pharm.

4.1. Program Specific Outcome:

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

PSO-1: Highlight advancements in knowledge associated with medicinal chemistry, Natural products chemistry, drug discovery, drug design and analytical techniques.

PSO-2: Independently carry out the design of bioactive molecules and synthetic research work.

PSO-3: Interpret the spectra of synthetic compounds, natural products and determine their structures.

PSO-4: Build professional, computational, analytical and critical thinking skills

PSO-5: Explain the unit operation and unit reactions in process chemistry

5. COURSE SPECIFICATION :

5.1.Course Identification and General Information

a. Course Title:	**Computer Aided Drug Design**	
b. Course Number/Code	**(MPC 203T)**	
c. Credit Hours	Theory	Practical
	04	NA
d. Study level/semester at which this course is offered	Sem II	
e. Pre-requisite	Stages of drug discovery, SAR, Rational design, Different techniques for drug discovery	
f. Co-requisite	Knowledge of Medicinal Chemistry subjects taught at B. Pharm and M Pharm first sem level	
g. Program in which the course is offered	M Pharm	
h. Language of teaching the course	English	
i. Prepared by	Dr. Santosh n Mokale	
j. Approved by HOD	Dr. K.G Baheti	

5.2.Course Description:

The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design.

5.3.Course Objectives:

- Role of CADD in drug discovery
- Different CADD techniques and their applications
- Various strategies to design and develop new drug like molecules.
- Working with molecular modeling softwares to design new drug molecules
- The in silico virtual screening protocols Peptidomimetics

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

(Use Bloom's Taxonomy words)

After completion of course, the student should be able to

CO Code	Course outcome
CO 203.01	Describe techniques and applications Quantitative Structure Activity Relationships
CO 203.02	Demonstrate QSAR, 3D-QSAR, contour map analysis and Statistical methods used in QSAR
CO 203.03	Relate Molecular Modeling, Docking and drug receptor interactions with drug
CO 203.04	Explain Molecular Properties, Drug Design concepts. Ppredict and analysed ADMET.
CO 203.05	Elaborate Pharmacophore Mapping and Virtual Screening.

6.1. Knowledge and Understanding

(Alignment of PSOs to COs)

Course Code	Program Specific Outcome				
	PSO-1	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO 203.01	H	H	L	H	-
CO 203.02	H	H	L	H	-
CO 203.03	H	H	L	H	-
CO 203.04	H	M	M	H	-
CO 203.05	H	M	L	H	-

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) Collaborative learning (Discussion) Project based Learning Blended learning Inquiry based learning Flash cards Video Equipment models	Formative Assessment Case study Class test Multiple choice questions Assignments Seminar Viva Voce Synopsis Tutorials Summative Assessment

6.3.Tools for the Teaching and learning

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

6.4.COURSE CONTENT

6.4.1. Theoretical Aspect:

Order	Topic list/units	Subtopics list	Number of Weeks	Contact Hours
1	**Unit I**	**Introduction to Computer Aided Drug Design (CADD)** History, different techniques and applications. Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi-substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters.	**03**	**12**
2	**Unit II**	**Quantitative Structure Activity Relationships : Applications**	**03**	**12**

		Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations. 3D-QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.		
3	**Unit III**	**Molecular Modeling and Docking** a) Molecular and Quantum Mechanics in drug design. b) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation c) Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE & BchE)	**03**	**12**
4	**Unit IV**	**Molecular Properties and Drug Design** **a)** Prediction and analysis of ADMET properties of new molecules and its importance in drug design. b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design. c) Homology modeling and generation of 3D-structure of protein.	**03**	**12**
5	**Unit V**	**Pharmacophore Mapping and Virtual Screening** Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping. In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols	**03**	**12**
	TOTAL		**15**	**60**

6.4.2. Practical Aspect

Sr.no	Practical	Number of Weeks
1	Synthesis of organic compounds by adapting different approaches involving (3 experiments) a) Oxidation b) Reduction/hydrogenation c) Nitration	**3**

2	Comparative study of synthesis of APIs/intermediates by different synthetic routes (2 experiments)	**2**
3	assignments on regulatory requirements in API (2 experiments)	**2**
5	Comparison of absorption spectra by UV and Wood ward – Fieser rule	**1**
5	Interpretation of organic compounds by FT-IR	**1**
6	Interpretation of organic compounds by NMR	**1**
7	Interpretation of organic compounds by MS	**1**
8	Determination of purity by DSC in pharmaceuticals	**1**
9	Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra	**1**
10	To carry out the preparation of following organic compounds	**1**
11	Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizine HCl).	**1**
12	Preparation of 4-iodotolene from p-toluidine.	**1**
13	NaBH4 reduction of vanillin to vanillyl alcohol	**1**
14	Preparation of umbelliferone by Pechhman reaction	**1**
15	Preparation of triphenyl imidazole	**1**
16	To perform the Microwave irradiated reactions of synthetic importance (Any two)	**1**
17	Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares	**1**
18	Calculation of ADMET properties of drug molecules and its analysis using softwares Pharmacophore modelling	**1**
19	2D-QSAR based experiments	**1**
20	3D-QSAR based experiments	**1**
21	Docking study-based experiment	**1**
22	Virtual screening based experiment	**1**

7.0.ASSESSMENT MECHANISM:

Sr. No.	Assessment Mechanism	Week due	Marks	Proportion of Final Assessment
1	Continuous Assessment (Theory)	2nd 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	**santoshmokale@rediffmail.com**

9.0.TEACHER'S AVAILABILITY FOR STUDENT SUPPORT:

Days	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
Time	**1:00-2:00**	**1:00-2:00**	**1:00-2:00**	**1:00-2:00**	**1:00-2:00**	**1:00-2:00**

10.0. LEARNING RESOURCES:

Sr.No.	Title of Learning Material	Details
1	Text books	1.Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers. 2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group.. 3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers. 4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis. 5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.

		6. Medicinal Chemistry by Burger, Wiley Publishing Co.
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 onlinequestionnaires

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	**Dr Santosh n Mokale**
Location	Department of Pharmaceutical Chemistry
Contact Detail (e-mail &cell no.)	santoshmokale@rediffmail.com, 9890409325
Office Hours	10:00 AM to 5:00 PM