COURSE TITLE	**COMPUTER AIDED-DRUG DESIGNING**
COURSE CODE	**01CB0501**
COURSE CREDITS	**4**

Objective:

1 The subject will make students expedite and enhance the drug discovery process by using computational methods to predict and optimize the interactions between potential drug candidates and biological targets.

Course Outcomes: After completion of this course, student will be able to:

1 Apply drug discovery principles to identify drug targets and leads.
2 Apply homology modeling and docking workflows for binding analysis.
3 Analyze ligand receptor interactions.
4 Analyze chemical formats, structures, and pharmacophore features for drug design.
5 Evaluate QSAR descriptors and predict biological activity of molecules.

Pre-requisite of course: Basic knowledge of Bioinformatics.

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
3	0	2	50	30	20	25	25

Contents : Unit	Topics	Contact Hours
1	**INTRODUCTION** Introduction to Drug Discovery and Drug Designing Process, History of drug development, basic pharmacodynamics, and pharmacokinetics, strategies for drug designing and development, and lead optimization	9
2	**FILE FORMATS** Small molecule rotation and string mapping: chemical nomenclature and notation like SMILE, ROSDAL string notation, protein 3-D structure file formats MOL, PDB, SDF.	9
3	**PHARMACOPHORES** Pharmacophores: Introduction, pharmacophore modeling, pharmacophore generation, hypogen theory, hip-hop theory.	8
4	**QSAR** QSAR (Quantity structure activity relationship): Historical development of QSAR, tools and technique of QSAR, parameter used in QSAR, application of QSAR, QSPR (quantity structure and property relationship).	8

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Contents : Unit	Topics	Contact Hours
5	**MODELLING AND DOCKING** Modeling and docking: History of homology modeling, assumption of homology modeling, homology modeling step, model validation, introduction to docking, types of docking, basic principle and method of docking.	8
Total Hours		**42**

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	**Module 1:** To analyze the small molecule from online databases	2
2	**Module 1:** To perform screening of the small molecules from the database for a particular category such as phenolic/acidic etc	2
3	**Module 1:** To generate the structure of chemical compounds using online tools	2
4	**Module 2 :** To generate the structure of chemical compounds using offline tools	2
5	**Module 2 :** To compare the file formats representing 2D and 3D structures and adjudicate their significance	2
6	**Module 3 :** To execute the process of downloading the 3D structure of a relevant protein to a certain disease from PDB	2
7	**Module 3 :** To analyze and compare the 3D structure using the visualization tools	2
8	**Module 3 :** To predict the physiochemical properties of the selected proteins	2
9	**Module 3 :** To predict the toxicity of proteins and chemical compounds	2
10	**Module 4 :** To classify the proteins based on ADME properties	2
11	**Module 4 :** To apply QSAR software for predicting the biological activity of chemical compounds/molecules	2
12	**Module 4 :** To perform the Installation of the virtual screening software	2
13	**Module 5 :** To compare and virtually screen the molecules for a given protein	2

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Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
14	**Module 5 :** To identify the drug-like molecules based on binding energy calculations	2
Total Hours		**28**

Textbook :

1 Bioinformatics. From Genomes to Drugs, Thomas Lengauer, Publisher Wiley, 2001

References:

1 Molecular Modeling-Principles and applications, Molecular Modeling-Principles and applications, Andrew R. Leach, , J. Chem. Inf. Comput, 2001

2 Fundamentals of Medicinal Chemistry, Fundamentals of Medicinal Chemistry, Gareth Thomas, Publisher Wiley, 2003

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery					
Remember / Knowledge	**Understand**	**Apply**	**Analyze**	**Evaluate**	**Higher order Thinking / Creative**
20.00	30.00	20.00	10.00	10.00	10.00

Instructional Method:

1 The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

2 The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.

3 Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.

Supplementary Resources:

1 Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory.

2 https://www.biopharmainstitute.com/course/CADDE

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