GUJARAT TECHNOLOGICAL UNIVERSITY

Syllabus for PG Diploma in Bioinformatics, Semester - 1

Subject Name: Computer-Aided Drug Design

Subject Code: 1310206 W.E.F 2021-22

1. Learning Outcomes

Learning Outcome Component	Learning Outcome (Learner will be able to)
Domain Knowledge	• Understands the fundamentals of Computer Aided-Drug Design.
Critical thinking, Logic Building, Problem Solving	• Developing & designing computer aided drugs and modelling 3D structures
Exposure and Cross-discipline Understanding	• Understanding the biochemical and statistical concepts with respect to Computer-Aided Drug Design.
Effective Communication	• Communicate ideas clearly and effectively
Professional & Ethical Behaviour	• Transparency, honesty and ethical reasoning in De novo Drug Design.

LO – PO Mapping: Correlation Levels:
1 = Slight (Low); 2 = Moderate (Medium); 3 = Substantial (High), "-"= no correlation

Sub Code: 1310206	PO1	PO2	PO3	PO4	PO5	PO6
LO1: Domain Knowledge	3	3	3	3	2	3
LO2:Critical thinking, Logic Building, Problem Solving	3	3	3	3	2	3
LO3:Exposure and Cross-discipline Understanding	3	3	3	3	2	3
LO4: Effective Communication	2	2	3	3	2	3
LO5: Professional & Ethical Behaviour	2	2	2	3	3	3

2. Course Duration: The course duration is 45 sessions of 60 minutes each.

3. Course Contents:

Module No:	Module Content	No. of Sessions	70 Marks (External Evaluation)
I	**Introduction to Computer Aided Drug Design (CADD)** History, different technique sand applications Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters, lipophilicity effects and parameters, steric effects (Taft steric and MR parameters) Experimental and theoretical	10	20

	approaches for the determination of these physicochemical parameters.		
2	**Quantitative Structure Activity Relationships** Applications 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.	9	10
3	**Molecular Modelling and Docking** Molecular and Quantum Mechanics in drug design, Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation, Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking.	10	20
4	**Molecular Properties and Drug Design** Prediction and analysis of ADMET properties of new molecules and its importance in drug design. 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. Homology modeling and generation of 3D-structure of protein.	8	10
5	**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.	8	10
6	**Introduction to Structure based Drug Design and process** 1. Layout of Docking and acquisition of target structure, Comparative modelling of protein (Homology modelling) Server based – PHYRE, SWISSMODEL etc. 2. Protein structure validation (ProSA), Ramachandran plot, assessment (RAMPAGE, Pdbsum, Procheck). 3. Active site/ Pocket identification – MetaPocket, CastP, Active site identification using	---	(30 marks CEC)

	4. PyMol,-Molecular Docking using Auto-Dock vina/Auto-Dock Tools/PyRx (For docking of multiple ligands), Protein and ligand preparation, Setting grid parameters and Docking parameters. 5. Docking analysis (based on binding energy, Hydrogen bond interactions, electrostatic interactions, hydrophobic interactions, etc.), Report construction 6. Introduction to Molecular Dynamics Simulations; Basic Principles of Molecular Dynamics Simulations (Non-bonded interactions, Bonding Potentials, Force fields), Molecular Dynamics Simulation using GROMACS, -Installation of software required for simulations, Definition of molecular structures, Force field and topology, Preparation of files, Simulation.		

4. Pedagogy:

- ICT enabled Classroom teaching
- Case study
- Practical/live assignment
- Interactive classroom discussions

5. Evaluation:

Students shall be evaluated on the following components:

	Internal Evaluation	**(Internal Assessment – 20 Marks)**
A	• Assignments	10 marks
	• Class Presence	5 marks
	• Record maintenance	5 marks
B	**Mid-Semester Examination**	**(Internal assessment-30 Marks)**
C	**End-Semester Examination**	**(External assessment-70 Marks)**

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6. Reference Books:

No	Author	Name of the Book	Publisher	Year of Publication / Edition
1	Robert M troud and Janet.F Moore	Computational and structural approaches to drug discovery	RCS Publishers	Latest edition
2	Y.C. Martin	Introduction to Quantitative Drug Design	Taylor & Francis.	Latest Edition
3	Ariens	Drug Design	Elsevier Publishers	Latest Edition
4	Smith and Williams	Principles of Drug Design	Taylor & Francis	Latest Edition
5	Richard B. Silverman	The Organic Chemistry of the Drug Design and Drug action	Elsevier Publishers	Latest Edition

Note: Wherever the standard books are not available for the topic appropriate print and online resources, journals and books published by different authors may be prescribed.

7. List of Journals/Periodicals/Magazines/Newspapers / Web resources, etc

- https://nptel.ac.in/courses/102106070
- https://www.springer.com/journal/10822
- https://github.com/volkamerlab/TeachOpenCADD.

Course Outcomes:

On completion of this course, students should be able to:

- Understand the basic concepts, terminology of molecular modeling, molecular docking and 3D QSAR.
- Gain working knowledge of different molecular modeling, molecular docking and 3D QSAR tools.
- Develop skills to study and analyze biological macromolecules in drug design framework.